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Detection of particles transported in weakly compressible fluids: mathematical models, analysis, and simulations

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Abstract

In this thesis, the problem of detecting small particles dispersed in air is considered. A method for the quantitative measurement of the particles, which is studied here, was developed at the research institute CAESAR in the course of the European integrated project NANOSAFE2. We investigate two issues: the transport of particles by air to a washing flask where the particles are being immersed in water and motion of particles in water flowing through a wet cell having an active boundary part responsible for the measurement.

For the transport of particles, a mathematical model that describes the evolution of the flow, the motion of dispersed particles, and the interaction between particles and air is derived. Thus, this model is related to a two-component flow problem. Under certain assumptions, the existence and uniqueness of weak solutions to the governing initial-boundary value problem on a non-empty time interval is shown. This result is established using a fixed-point technique.

For the measurement of particles, we first derive a coupled initial-boundary value problem that describes the evolution of the flow, particle density, and surface mass density of measured particles, and the interaction between particles and water. The surface mass density of measured particles is described via a boundary condition of hysteresis type on the particle density posed on the active part of the wet cell. To investigate the derived model theoretically, the influence of the particles on the water is neglected. Thereby the whole problem is divided into two sub-problems, the flow problem and the evolution of particle density, so that the velocity and pressure can be found independently of the particle density. The existence of weak solutions is proved on a non-empty time interval determined by the data of the flow problem. The uniqueness is proved under the assumption that the divergence of the velocity field is essentially bounded. The existence and uniqueness of weak solutions to the evolution of the particle density can be shown in the case of arbitrary finite time intervals, provided that the velocity field is sufficiently regular.

Finally, the numerical simulation of the model of measurement in the case of full coupling is described. We propose a scheme for the numerical solution of the model equations using the finite element method. The numerical behavior of the proposed scheme is discussed for some selected examples. First simulations of the measurement in the wet cell in two and three dimensions are presented.

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Contents

1 Introduction

The present thesis is devoted to the detection of small particles. This problem has been studied at the research institute CAESAR in the course of the European integrated project NANOSAFE2 – Safe production and use of nanomaterials. Within the project, CAESAR investigated the possibility of capturing and detecting nanoparticles immersed in aqueous solvents by means of techniques based on specifically binding peptides, see [69]. We will focus on two components of the developed technique and consider mathematical modeling and analysis of the derived models. We will then present results of numerical simulations of one of these models.

We will distinguish the problems of detection and pure transport of particles in a flowing medium. The reason for this distinction is that the detection procedure developed at CAESAR is divided into two sub-processes: the washing out of particles and their measurement. These two sub-processes explained in Section 1.2 are modeled in different ways.

This chapter is structured as follows: the motivation is given in Section 1.1, the detection method developed at CAESAR is described in Section 1.2. Some conventional models and methods are reviewed in Section 1.3, and the objectives of the thesis and the contents of the following chapters are summarized in Section 1.4.

1.1 Motivation

The detection of particles gained special interest in the last decades when the possibilities of nanotechnology were discovered. The ability to tailor material properties at nanoscale enabled the engineering of novel materials that have entirely new properties, which led to new research areas and to the development of new commercially available products. With only a reduction of size the fundamental characteristics of substances such as electrical conductivity, colour, strength, and melting point – properties which are usually considered constant for a given material – can all change. Therefore, nanomaterials show promising application potentials in a variety of fields such as chemistry, electronics, medicine, cosmetics or the food sector. For example, metal oxide nanopowders have found already increasing applications in commercial products like sunscreens, cosmetics, catalysts, functional coatings, medical agents, etc.

However, not only its large potential was recognized but also sceptical voices concerning nanotechnology could be heard in public. One of the sharpest critics of industrial nanoparticle applications is the non-governmental organisation ETC Group. However, the fear of risk associated with nanoparticle use was mainly caused by limited scientific knowledge about potential side effects of nanoparticles in the human body and the environment due to their special properties. They may, for example, penetrate into body cells and break through the blood-brain barrier [42]. See also [68].

The objectives of the European project NANOSAFE were to assemble available information from public and private sources on chances and possible hazards involving industrial nanoparticle production, to evaluate the risks to workers, consumers and the environment, and to give recommendations for setting up regulatory measures and codes of good practice to obviate any danger [42]. The research on nanoparticles was continued in a second project, NANOSAFE2. Within NANOSAFE2, 25 partners from industry, research centers and universities work on four sub-projects: detection and characterization techniques, health hazard assessment, and development of secure industrial production systems and safe applications, societal and environmental aspects.

As one of the participants, the research institute CAESAR has developed a peptide based biosensor for detecting nanoparticles. Besides this approach, other detection methods have been investigated, for example, light scattering-based techniques or techniques based on different physical principles such as electrostatics, thermophoresis, bubbling, vapour condensation, etc. [70].

In the present thesis, two steps of the detection procedure developed at CAESAR will be considered from the mathematical point of view. We will derive mathematical models to describe the physical processes, analyse the solvability issue, and present simulation results for one of the derived models. Before describing the detection plant we are going to model, we mention some "classical applications" of nanomaterials.

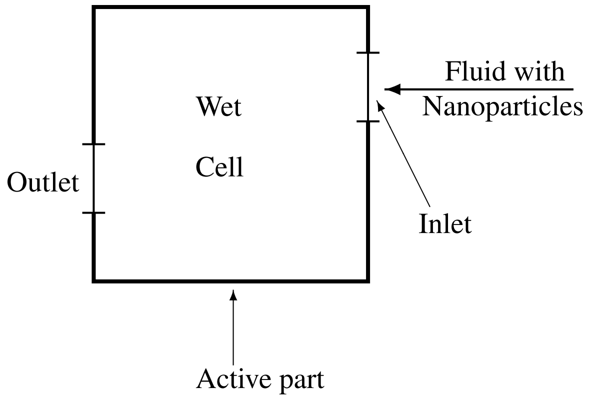
The particular properties of small particles have been exploited by humans since prehistory but without specific knowledge. Famous and perhaps surprising examples are objects made of clay, a highly stable blue pigment the Mayas used to paint their figures, Damascus blades, or the brilliant red colour of some church windows.

Clay largely consists of the mineral kaolinite, which has the structure of thin platelets, only a few tens of nanometers thick. These slide readily over each other when the mineral has absorbed water whereby clay becomes smeary and easily shapeable. From the eighth century on the Mayas were able to paint their clay figures with a blue pigment that could resist the ravages of time. They synthesized an inorganic-organic nanocomposite consisting of palygorskite, another clay mineral also known as "mountain leather", and an organic indigo pigment. This highly stable old pigment is now again being produced in the USA by MCI Mayan Pigments, Inc. Damascus blades were renown in the Middle Ages for their filigree markings, their sharpness, and their fracture toughness. For a long time modern metallurgy could not find a scientific explanation for these properties. Only at the end of 2006, carbon nanotubes could be found in the blades. This nanowire reinforcement at least explains their fracture toughness. In the Middle Ages church windows were coloured using an extremely fine, nano-scale dispersion of gold. This causes a brilliant red colour that endures for centuries [53].

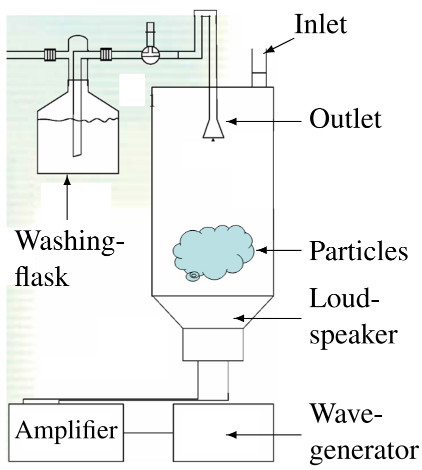
1.2 Description of the detection procedure

Figure 1.2.1 shows schematically a device developed at CAESAR for the detection of particles. The considered device was constructed in particular to specifically detect large organic molecules in air. An organic molecule is a chain consisting of many links connected by flexible bonds so that the molecule can assume different configurations.

Before such particles can be detected, they are prepared as shown in Figure 1.2.1.b. Air containing particles is injected into a vessel. The air flow from the inlet to the outlet transports the particles into the water quench of a washing flask. Concurrently a loudspeaker generates acoustic waves to prevent the particles from the deposition on the bottom of the vessel. In the washing flask, the particles are washed out of the air into the water when the air bubbles rise to the water surface. After a certain time, the water contains a significant amount of particles, and



1.2.1.a: Scheme of the measurement



1.2.1.b: Preparation: Washing out

Figure 1.2.1: Scheme of the device constructed for the detection of particles

the obtained dispersion is fed into a biosensor where the particles are detected.

As shown in Figure 1.2.1.a, the sensor consists of a wet cell having an active boundary part providing the measurement. When the dispersion flows through the wet cell, the particles arriving at the active part are trapped until the sensor is saturated. The trapped mass can be measured, and the concentration of particles in the dispersion can be estimated.

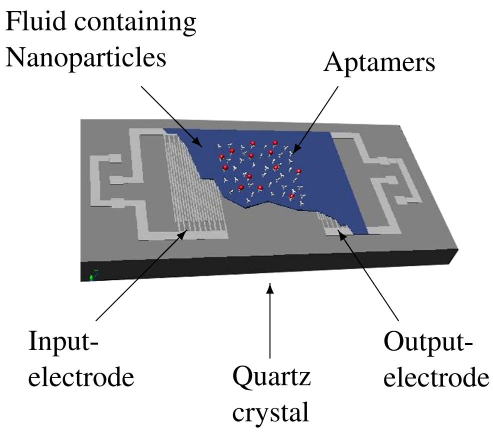


Figure 1.2.2: Scheme of the active part

A schematic sketch of the active part is shown Figure 1.2.2. In order to detect the particles, special molecules, called aptamers, are immobilized on a quartz crystal by means of excitation and detection electrodes. Free ends of the aptamers are receptors that can specifically bind particles form the immersion. Once a particle is attached to an aptamer, it cannot be released anymore. To measure the amount of trapped particles, acoustic shear waves are generated by the excitation electrodes via piezoelectric excitation. The change of the surface mass load causes a phase change in the waves travelling along the aptamer layer, and this phase change can be measured by the detection electrodes.

1.3 Brief overview of conventional models and methods

From the description of the detection method in Section 1.2, it is clear that many interesting and challenging issues related to the whole detection plant (see Figure 1.2.1) or parts of it can be considered to get a better understanding of the physical processes occurring during the measurement. The aim of this section is to describe briefly some conventional notions, models and methods that we consider interesting as a general state of knowledge. However, not all of these topics are directly applicable to the problem considered in the present thesis.

Evolution of mixtures. One topic which is definitely related to the device shown in Figure 1.2.1 is the flow of mixtures. As described in Section 1.2, the fluids flowing through each unit of the detection plant consist of at least two components: an air-particle mixture in the vessel, a water-particle mixture in the wet cell, and an air-water-particle mixture in the washing flask. A variety of models for the description of multi-component flow have been developed because each mixture shows specific properties. There are even mixtures where different derivations of governing equations yield different results. An example of such a case will be given below for a mixture of discrete particles contained in a continuum fluid.

But also for "simple mixtures" consisting of two continuum components, several scenarios can be distinguished: the components can be miscible (up to certain proportions) or immiscible. For example, ethyl alcohol and aqueous salt solutions (sulphates of zinc, copper, etc.) are miscible in all proportions (see [33, X.3]), whereas water and oil are immiscible. Important situations where the flow of immiscible liquids occurs are, for example, oil recovery, lubricated pipelining, etc. An essential difference between mixtures of immiscible and miscible fluids are diffusive effects occurring when miscible fluids come in contact with each other. Thus, even if no outer force or pressure gradient is applied, the mixture can be in a dynamical state due to the composition gradient.

One possibility to describe the flow of miscible liquids is to derive a system of equations in terms of variables such as the volume fraction of one of the components ϕ, mixture density ρ, mass averaged velocity $\boldsymbol{U}$, mixture pressure p, and temperature θ. The system consists of a continuity equation for ρ, $\boldsymbol{U}$, a drift diffusion equation for ϕ, $\boldsymbol{U}$, equations of motion for ρ, $\boldsymbol{U}$, p (and possibly ϕ, depending on the stress tensor), and an energy equation for θ.

The stress induced by the composition gradient or density gradients can be modeled using the Korteweg stress, or the traceless version of it. The Korteweg tensor is given by the formula (see [33, X.3, X.4])

$$T_{ij}^K = \delta_1 \frac{\partial \rho}{\partial x_i}\frac{\partial \rho}{\partial x_j} + \delta_2 \frac{\partial \phi}{\partial x_i}\frac{\partial \phi}{\partial x_j} + \gamma_1 \frac{\partial^2 \rho}{\partial x_i \partial x_j} + \gamma_2 \frac{\partial^2 \phi}{\partial x_i \partial x_j} + \gamma_3 \left(\frac{\partial \rho}{\partial x_i}\frac{\partial \phi}{\partial x_j} + \frac{\partial \phi}{\partial x_i}\frac{\partial \rho}{\partial x_j} \right). \quad (1.1)$$

The situation becomes even more complicated if phase changes have to be considered. A detailed derivation of models for (im)miscible multi-component and/or multi-phase flows, solution techniques and extensive lists of possible applications can be found, for example, in books [32, 33, 13]. The evolution of mixtures of (dilute) gases can also be described by Boltzmann equations for multiple species [11, 12].

Next, we mention briefly the example where different derivations of governing equations yield different results for the same mixture. Following [31], we consider an incompressible fluid-particle suspension and compare the equations given by mixture theory and ensemble averaging. Let ρ, $\boldsymbol{V}$, P, $\mathbb{T}^*$ be the true density, velocity, pressure, and stress in the mixture, and let the indices s, f indicate variables of the solids and the fluid, respectively. Further denote the solids fraction by ϕ and the fluids fraction by $\epsilon = 1 - \phi$. If body forces are neglected, the classical equations of mixture theory for two incompressible constituents are given by

$$\begin{aligned} \epsilon_t + \operatorname{div}(\epsilon\,\boldsymbol{v}_f) &= 0, \\ \phi_t + \operatorname{div}(\phi\,\boldsymbol{v}_s) &= 0, \\ \overline{\rho_f}\left[(\epsilon\,\boldsymbol{v}_f)_t + \operatorname{div}(\epsilon\,\boldsymbol{v}_f \otimes \boldsymbol{v}_f)\right] &= \boldsymbol{m}_f + \operatorname{div}\mathbb{T}_f \\ \overline{\rho_s}\left[(\phi\,\boldsymbol{v}_s)_t + \operatorname{div}(\phi\,\boldsymbol{v}_s \otimes \boldsymbol{v}_s)\right] &= \boldsymbol{m}_s + \operatorname{div}\mathbb{T}_s, \\ \boldsymbol{m}_f + \boldsymbol{m}_s &= \operatorname{div}\mathbb{S}, \end{aligned} \tag{1.2}$$

where $\boldsymbol{m}_f$, $\boldsymbol{m}_s$ are the forces of interaction between the constituents and $\mathbb{S}$ is an interaction stress.

Two fluid equations can also be derived by ensemble averaging. In this approach one defines the indicator function

$$H(\boldsymbol{x}) = \begin{cases} 0 & \text{if } \boldsymbol{x} \text{ is in solid,} \\ 1 & \text{if } \boldsymbol{x} \text{ is in fluid,} \end{cases}$$

and $<>$ designates the operation of taking the average over many identical trials at $\boldsymbol{x}$ at time t. Then the fluid and solid fractions are given by

$$\begin{aligned} \langle H\rangle &= \epsilon(\boldsymbol{x},t) = 1 - \phi(\boldsymbol{x},t), \\ \langle 1 - H\rangle &= 1 - \langle H\rangle = \phi(\boldsymbol{x},t). \end{aligned}$$

If $\boldsymbol{V}(\boldsymbol{x},t)$ is the true velocity, then the averaged fluid and solid velocities $\boldsymbol{V}_f$ and $\boldsymbol{V}_s$, are given by

$$\boldsymbol{V}_f = \frac{\langle H\,\boldsymbol{V}\rangle}{\langle H\rangle} = \frac{\langle H\,\boldsymbol{V}\rangle}{\epsilon}, \qquad \boldsymbol{V}_s = \frac{\langle (1-H)\boldsymbol{V}\rangle}{\phi}.$$

The composite and mass averages for a quantity f are defined by

$$\begin{aligned} f_c &= \langle f\rangle = \epsilon\, f_f + \phi\, f_s, \\ f_m &= \frac{\langle \rho\, f\rangle}{\langle \rho\rangle} = \frac{(\rho\, f)_c}{\epsilon\,\rho_f + \phi\,\rho_s}. \end{aligned}$$

To formulate the equations of motion, we additionally introduce a one-dimensional Dirac's delta function $\delta_\Sigma(\boldsymbol{x})$ across the solid-fluid interface. Let $\boldsymbol{\nu}$ be the outward normal to the solid, and $\mathbb{T}^* \cdot \boldsymbol{\nu} = \boldsymbol{t}$ the traction. Then the following equations can be derived (body forces are neglected again)

$$\begin{aligned} \epsilon_t + \operatorname{div}(\epsilon\,\boldsymbol{V}_f) &= 0, \\ \phi_t + \operatorname{div}(\phi\,\boldsymbol{V}_s) &= 0, \\ (\rho_c)_t + \operatorname{div}(\rho_c\,\boldsymbol{V}_m) &= 0, \\ \overline{\rho_f}\left[(\epsilon\,\boldsymbol{V}_f)_t + \operatorname{div}\langle H\,\boldsymbol{V}\,\boldsymbol{V}\rangle\right] &= \operatorname{div}\left(\epsilon\,\mathbb{T}^*_f\right) - \langle \delta_\Sigma\,\boldsymbol{t}\rangle, \\ \overline{\rho_s}\left[(\phi\,\boldsymbol{V}_s)_t + \operatorname{div}\langle (1-H)\boldsymbol{V}\,\boldsymbol{V}\rangle\right] &= \operatorname{div}\left(\phi\,\mathbb{T}^*_s\right) + \langle \delta_\Sigma\,\boldsymbol{t}\rangle. \end{aligned} \tag{1.3}$$

Supposing that mixture theory and ensemble averaging yield the same results and comparing the systems (1.2) and (1.3), we get the relations

$$\begin{aligned} &\boldsymbol{V}_f = \boldsymbol{v}_f, \;\; \boldsymbol{V}_s = \boldsymbol{v}_s, \;\; \epsilon\,\mathbb{T}_f^* = \mathbb{T}_f, \;\; \phi\,\mathbb{T}_s^* = \mathbb{T}_s, \\ &\boldsymbol{m}_f = \overline{\rho_f}\,\mathrm{div}\,(\epsilon\,\boldsymbol{v}_f \otimes \boldsymbol{v}_f - \langle H\,\boldsymbol{V} \otimes \boldsymbol{V}\rangle) - \langle \delta_\Sigma\,\boldsymbol{t}\rangle, \\ &\boldsymbol{m}_s = \overline{\rho_s}\,\mathrm{div}\,(\phi\,\boldsymbol{v}_s \otimes \boldsymbol{v}_s - \langle (1-H)\boldsymbol{V} \otimes \boldsymbol{V}\rangle) + \langle \delta_\Sigma\,\boldsymbol{t}\rangle, \\ &\mathrm{div}\,\mathbb{S} = \mathrm{div}\Big(\overline{\rho_f}\,\epsilon\,\boldsymbol{v}_f \otimes \boldsymbol{v}_f + \overline{\rho_s}\,\phi\,\boldsymbol{v}_s \otimes \boldsymbol{v}_s - \big\langle\, [\overline{\rho_f}\,H + \overline{\rho_s}(1-H)]\,\boldsymbol{V} \otimes \boldsymbol{V}\big\rangle\Big). \end{aligned} \tag{1.4}$$

Still, there is no contradiction between the equations of mixture theory and the ensemble averaged equations.

Now, assume that the fluid phase is Newtonian,

$$\mathbb{T}^* = -P\,\mathbb{I} + 2\,\mu\,\mathbb{D}[\boldsymbol{V}] \qquad \text{in the fluid,}$$

and the solid phase is a rigid body for which

$$\mathbb{D}[\boldsymbol{V}] = 0 \qquad \text{on solids,}$$

where $\mathbb{D}[\boldsymbol{V}] = \frac{1}{2}\left(\nabla\boldsymbol{V} + [\nabla\boldsymbol{V}]^T\right)$ is the rate of strain.

The stress for the fluid phase in mixture theory is given by

$$\mathbb{T}_f = -\epsilon\,p_f\,\mathbb{I} + 2\,\epsilon\,\mu\,\mathbb{D}[\boldsymbol{v}_f].$$

This differs from the fluid stress obtained from ensemble averaging

$$\mathbb{T}_f = \epsilon\,\mathbb{T}_f^* = \langle H\,\mathbb{T}^*\rangle = -\epsilon\,p_f\,\mathbb{I} + 2\,\epsilon\,\mu\,\mathbb{D}[\boldsymbol{v}_c].$$

Here, the ensemble averaged pressure in the liquid (P_f) is identified with the liquid pressure in mixture theory, i.e. $P_f = \langle H\,P\rangle/\epsilon = p_f$.

Finally, note that other averaging procedures are possible, and, for example, soft spatial averaging yields the same result for the stress tensor in the fluid as in the case of ensemble averaging, see [31]. A similar averaging method will be used in Sections 2.4.4 and 3.3 to regularize the velocity field in the continuity equation for the particles.

Single-Phase Flow. Similar to the case of mixtures, divers models exist also for one-component flows. One can distinguish between incompressible and compressible fluids (liquids and gases), and the compressible ones can be regarded as inviscid (called Euler or ideal fluids) or viscous and thermally conducting (Navier-Stokes-Fourier fluids). Further refinements are possible. Differences between the corresponding models consist in the number of variables used to describe the flow, and the state equations, which are necessary to close the models.

Let us note that the consideration of the flow of a single Newtonian phase is a challenging issue concerning the mathematical analysis and numerical computations. To substantiate this statement we refer to the preface of [40] where we can find the quote: “More than two centuries after this introduction by L. Euler (and later by Navier) of the fluid mechanics equations, much remains to be understood mathematically even if considerable progress has been (slowly) made.” As for the numerical side, see the introduction in [19]: “Many times significant errors have been made when using CFD software packages without a solid background in fluid mechanics and numerical analysis." The abbreviation CFD stands for computational fluid dynamics. We will not go into details but mention that, for certain applications in CFD, the parallelization is very important to reduce the running time for realistic simulations in large domains on fine grids.

The reader interested in mathematical or computational methods for single-phase flows is referred to books [17, 18, 19, 36, 38, 40, 41, 47, 60].

Aptamers. Aptamers are oligonucleic acid or peptide molecules that bind to a specific target. Besides their application in the biosensor shown in Figure 1.2.2, they can be used in a variety of biochemical and clinical applications. Let us mention a few of them to indicate their potential.

Biochemical applications of aptamers are, for example, the identification of biomolecules that can point out various diseases. It is possible to select aptamers that bind to a specific cell type or subpopulation of malignant cells (for example, tumor cells), and, in individual cases, they have already been used successfully to inhibit the virulence of such targeted microorganisms. Such a potential inhibition property makes aptamers in particular useful to validate the function of their targets in cell-culture experiments and in vivo. These and other possible applications are discussed in [44].

Further applications of aptamers include the inhibition of human thrombins [7], synchronous cancer imaging, therapy, and sensing of drug delivery [5], the replacement of antibodies in diagnostics [30], the application of peptide atpamers in molecular medicine [29], and the application as therapeutics [46].

The binding property with high specificity to the target is already exploited during the production of aptamers. Aptamers are produced by systematic evolution of ligands by exponential enrichment (SELEX) process. In this process first a combinatorial nucleic acid library (DNA or RNA) with a large number of random sequences is synthesized. The library is then incubated with the desired target molecule under conditions suitable for binding. Next the unbound nucleic acids are partitioned from those bound specifically to the target molecule which are then eluted from the target molecule and amplified. This procedure is reiterated until the resulting sequences are highly enriched [26, 67]. An early description of aptamer production can be found in [15, 7], and further description of the separation methods used in SELEX in [24].

The active part. Finally, we note that Figure 1.2.2 is a simplified scheme of an acoustic wave sensor. A more thorough description of the mathematical modeling, analysis and numerical simulation can be found in [50].

1.4 Objectives and description of the results obtained

In this thesis we consider processes occurring in the vessel and the wet cell shown in Figure 1.2.1. The objectives of the thesis include the following three aspects: mathematical modeling, analysis and numerical simulations. This means, our overall goal is to derive mathematical models that have the following features.

- They describe the evolution of the particles in the flowing medium and, in case of the wet cell, the amount of particles bound by the active part.

- They are formulated as initial-boundary value problems for which the well-posedness, at least the existence and uniqueness of generalized solutions, can be established.
- They can be solved numerically without “too high programming and computing efforts”.

As we will consider models that have such features, it is clear that we cannot use the models described in Section 1.3 in their full strength. Let us mention some of the difficulties. If the equations of mixture theory were used, the Korteweg tensor (1.1) should to be included in the stress term of the momentum equations. This causes problems in the mathematical analysis, because we do not know how to derive suitable a priori estimates in this case.

If averaged equations were used, further modeling or guessing is necessary, as the system is not closed. Considering ensemble averaging, for example, we see that the relations (1.4) contain averages of products, which cannot be directly identified with macroscopic variables. The ensemble average of a product is not the product of ensemble averages, so that these terms need further modeling [31, 33].

For these reasons, we will consider simpler models than those mentioned in Section 1.3. In the following, the vessel will be referred to as “the transport part” and the wet cell as “the measurement part”. Thus, the model related to a system of governing equations with initial and boundary conditions for the transport part is called “transport problem”. The model of the measurement part is called “coupled measurement problem” or “decoupled measurement problem” depending on the accounting for the mutual interaction between the particles and the fluid. The term “decoupled" means that the problem consists of two subproblems: the “flow problem” and the “evolution of the particle density”, where the motion of particles does not affect the total flow.

All models are formulated as initial boundary value problems in such a way that the amount of particles which leaves the vessel or wet cell, or adhere to the active part of the wet cell, is determined by the amount of particles entering the plant.

The present thesis is divided into three parts: the derivation of mathematical models, their theoretical investigation, and numerical simulations. First, we derive fully coupled equations for the transport and measurement problems. Then we introduce certain simplifications to obtain a relaxed transport problem and a decoupled measurement problem. For these problems we will show the existence and uniqueness of generalized solutions. Finally, the coupled measurement problem will be solved numerically.

The Subsections 1.4.1, 1.4.2, and 1.4.3 summarize the content of the subsequent chapters.

1.4.1 Derivation of mathematical models

Chapter 2 is devoted to the derivation of the mathematical models. Starting with the consideration of compressible Newtonian fluids we introduce the concept of weak compressibility to obtain a system of partial differential equations that, in combination with initial and boundary conditions, is called the flow problem. It is formulated in (2.1). The equations look similar to the Navier-Stokes equations for incompressible fluids. The difference is that small volume changes are included in the model instead of assuming complete incompressibility.

For the description of the transport of particles, we will first derive the system of equations (2.46). It consists of two continuity equations, one for each component, and $2N$ equations of motion, where N is the dimension of the considered space. The interaction between the components is modeled by interaction terms in the equations of motion. To derive the equations we first average the equations for the velocity of single particles presented in [64] to obtain the momentum conservation for the particle flow. Using results on the Boltzmann equations for mixtures, we obtain a continuity equation for the particle flow and an expression for the influence of the particle flow on the liquid flow. To this end, simplifying assumptions on the stress tensor are necessary.

For theoretical investigations, we simplify the above sketched equations for the transport of particles by using expansion with respect to a small parameter and regularizing the velocity field in the continuity equation for the particle flow. Thereby the velocity of particle flow is eliminated, and the resulting system of equations consists of two mass conservations and a global momentum conservation both for the particle and fluid flow. The equations are given in (2.2).

For the measurement of particles, the equations describing the coupled measurement problem are given in (2.3). The system of equations consists of the mass conservation law for weakly compressible liquids, the mass conservation for the particle flow in the form of drift diffusion equation, and the global momentum conservation (particles and fluid). The surface density of adhered particles on the active part of the wet cell is an additional unknown, which is necessary to describe a boundary condition of hysteresis type on the active part of the wet cell.

To derive this special boundary condition, the mass flux of particles arriving at the active part is related to the rate of change of the surface mass density of adhered particles. The properties of the aptamers, non-detachment of adhered particles and saturation if all aptamers are occupied, are modeled a boundary operator of hysteresis type, see (2.54).

The conservation equation for the particles is derived using Smoluchowski's approximation for the Langevin equations. This results in a drift diffusion equation for the particle density, where the drift is determined by the velocity of the ambient liquid. Thereby, the mass flux of particles towards the active part of the wet cell is given in terms of the gradient of the particle density. Completed with boundary conditions on the inlet, outlet and solid walls of the wet cell, the derived problem is called evolution of the particle density (2.5). Combining the evolution of the particle density with the flow problem (to obtain the velocity of the liquid) yields the decoupled measurement problem (2.4). This problem will be used for theoretical investigations.

To include the influence of the particles on the liquid we use the conservation of the total momentum as prescribed by mixture theory. Additionally, we can identify the mixture theory variables with the ones used for the decoupled model. Finally, we obtain practically the same structure of the equations as in the case of decoupling. The sole difference is an additional convective term appearing in the momentum equation and describing the influence of the particle flow on the fluid. This coupled measurement problem will be investigated numerically.

1.4.2 Theoretical investigations

Chapter 3 contains the theoretical part of this thesis. It is devoted to the investigation of the transport problem (see Section 3.3), and the decoupled measurement problem (see Section 3.4). The latter one is split into the flow problem and the evolution of the particle density. Therefore the transport problem, the flow problem, and the evolution of the particle density will be considered separately.

For each of these three problems, we prove the existence and uniqueness of weak solutions. The existence of weak solutions for the decoupled measurement problem follows from the existence results on the flow problem and the evolution of the particle density. To obtain the uniqueness of solutions, we have to assume additional regularity of the solutions of the flow problem.

The transport problem is considered in Section 3.3. This problem consists of the continuity equations for each component, a global momentum conservation, initial values for the pressure, velocity, particle density, and Dirichlet boundary conditions for the velocity. We prove the existence of a non-empty time interval such that the problem admits unique weak solutions under the following requirements: The considered domain $\Omega \subset \mathbb{R}^N$ is bounded and has a $\mathcal{C}^2$ boundary, the initial functions for the pressure and velocity are in $H^1(\Omega)$ and $H^1(\Omega)^N$, respectively, the initial value of the particle density is Lipschitz continuous with its support being separated from the boundary by a positive distance, and the boundary value of the velocity is the trace of an $H^2(\Omega)^N$-function. For the precise formulation see Definition 3.3.1 and Theorem 3.3.2.

The flow problem is considered in Section 3.4.1. It consists of the continuity equation, the equations of motion and Dirichlet boundary conditions for the velocity. For this problem, we show the existence of a non-empty time interval on which unique weak solutions exist. This problem seems simpler than the previous one but the treatment of the evolution of the particle density requires more regularity of the velocity field. In order to obtain a sufficiently regular solution, we suppose that the initial value of the pressure is in $H^1(\Omega)$, the initial value of the velocity in $H^2(\Omega)^N$, and the boundary value for the velocity is the trace of an $H^2(\Omega)^N$-function. Again, we assume that the domain $\Omega \subset \mathbb{R}^N$ is bounded and has a $\mathcal{C}^2$ boundary. See Definition 3.4.2 and Theorem 3.4.4 for the precise result.

The evolution of the particle density problem is investigated in Section 3.4.2. This problem consists of a drift-diffusion equation, initial values for the particle density and the surface mass density of adhered particles, a Neumann-type boundary condition on the outlet and solid boundary of the wet cell, a Robin-type boundary condition on the inlet, and a boundary condition of hysteresis type at the active part that relates the particle density to the surface mass density. This problem will be considered for $H^1(\Omega)$-initial values and constant-in-time inflow of particles through the inlet. In contrast to the other problems, we show the existence and uniqueness of weak solutions in bounded Lipschitz domains on arbitrary time intervals provided the velocity field is sufficiently regular. The results obtained on the flow problem guarantee sufficient regularity for the existence of weak solutions. As for the uniqueness it can be proved under stronger assumptions. See Definition 3.4.19 and Theorem 3.4.21 for the exact formulation. An important tool to investigate the evolution of the particle density is a special embedding theorem in anisotropic Sobolev spaces, see Definition 3.4.33 and Theorem 3.4.34. The embedding was communicated to me by Pavel Krejčí.

Finally, Theorem 3.4.1, which is a consequence of Theorems 3.4.4 and 3.4.21, states the main result for the decoupled measurement problem.

1.4.3 Numerical computations

In Chapter 4, the coupled measurement problem is solved numerically. We decided to consider this problem because of the following aspects: The structure of the system is consistent with other conventional theories, it is still close to the decoupled measurement problem that can be analyzed theoretically (see Section 3.4), the nonlinear boundary condition makes it an interesting problem, and it can be treated numerically using conforming finite elements (FE).

To explain the first aspect, we notice that the system of equations in the coupled measurement problem is similar to the equations of mixture theory and to the macroscopic balance equations derived from Boltzmann equations for mixtures. That is, the system consists of continuity equations for each component and the conservation of the total momentum. In contrast, the decoupled measurement problem contains only the influence of the liquid on the particles, and therefore, only the momentum of the liquid is conserved.

Since the evolution of the particles is described via a diffusion equation, conforming FE are appropriate for the numerical treatment of the coupled measurement problem, at least, if the diffusion coefficient is large and the discretization is sufficiently fine. Here, continuous piecewise linear shape functions will be used on a triangular (tetrahedral) mesh in two (three) dimensions. This method is not suitable for the numerical solution of the transport problem, where the hyperbolic continuity equation appears. To solve such equations, different FE techniques, for example, streamline diffusion, Galerkin least squares or discontinuous Galerkin FEM, or other discretization methods like finite difference or finite volume methods are necessary, see [19, Chapters 3,4].

In Section 4.1 we present a discretization scheme for the coupled measurement problem. The scheme is split into the computation of the variables corresponding to the fluid flow (velocity and pressure), and the variables corresponding to the particles (volume density and surface density on the active part of the wet cell). The reason for this separation is twofold. First, the computation of the particle variables requires an iterative method because of the nonlinear boundary condition on the active part of the wet cell. Second, numerical computations show that a small time step in the discretization of the particle variables is necessary to avoid (or at least to dampen) oscillations. This effect can be explained as follows. In the terminology of [19, Section 4.1.9], the decoupled measurement problem becomes singularly perturbed for diffusion coefficients in the range given by Table 2.6.4, thus a sufficiently fine discretization is necessary to avoid the Gibbs phenomenon. Further, regarding the beginning of Section 4.2 in connection with Lemma 3.4.22, we see that a bound on the time step for the particle variables in terms of the diffusion coefficient already occurs during the theoretical investigation of the evolution of the particle density. Therefore, computational effort can be saved if the flow variables are not computed in every time step. The scheme is implemented in Scheme 4.1.1, page 119.

Finally, numerical results will be presented in Section 4.2. The computations are carried out using the FE program Felics which is developed at the Chair of Mathematical Modeling at Technische Universität München. The first example in Section 4.2.1 considers a closed wet cell, where the drift velocity is set to zero. It illustrates the sensitivity of the proposed scheme with respect to the time step length, and we propose a regularization of the hysteresis boundary condition that enables us to use larger time steps. This is useful when physically realistic scenarios are considered.

Next, the flow of particles through an open wet cell without any active part is considered in Section 4.2.2. It occurs that the main stream of particles leaves the wet cell and almost no particles arrive at the boundary. Thus, in subsequent examples, the active part will be positioned on an obstacle in the interior of the wet cell.

In Sections 4.2.3 and 4.2.4, simulations of a wet cell are presented in two and three dimensions, respectively. Since the diffusion coefficient of particles in water is extremely small ($< 10^{-16}\ \mathrm{m} \cdot \mathrm{s}^{-2}$, see Table 2.6.4), stabilization techniques are necessary to obtain realistic results in this case. To avoid such difficulties, we consider air instead of water, which provides, for example, the diffusion coefficient $5.31 \cdot 10^{-8}\ \mathrm{m} \cdot \mathrm{s}^{-2}$ for spherical titanium dioxide particles of diameter $0.01\ \mu\mathrm{m}$.

2 Derivation of mathematical models

In this chapter, we give the mathematical formulation of the models discussed in Chapter 1. They describe the evolution of a two-component mixture. The air in the vessel or the water in the wet cell considered as conventional fluids will be referred as the first component or phase. The particles will be considered as a special dilute fluid and referred as the second component or phase. In contrast to water or air, the particles are assumed to be rarefied enough so that they do not exert pressure or stress on each other.

Similar to [17, 18, 47, 40, 58] we consider the flow under the continuum hypothesis. This means that the smallest considered parts of the material are so called “fluid particles”, see e.g. [58, 1.1]. A fluid particle is not a rigid particle but an ensemble of molecules. Such an ensemble has to contain enough molecules to ensure a proper averaging of physical quantities. On the other hand, it has to be small compared to the region where the flow is considered so that macroscopic quantities like density, velocity or temperature can be viewed as continuous functions of points associated with fluid particles.

Analogously to the method of fluid particles, we will describe the solid particle medium as a continuum consisting of small volumes, where each volume contains sufficiently large number of solid particles. It should be noted that the points of this continuum are sufficiently "larger" than those for the fluid continuum because there are much more molecules than particles in a fixed volume. Therefore, we may average fluid-related physical quantities appearing in equations for particle flows.

This chapter is structured as follows. In Section 2.1, the notation is given. Section 2.2 presents (without derivation but just for reference) mathematical formulations of all models considered in the thesis. The derivation is given later. In Section 2.3, the motion of weakly compressible fluids is considered, and equations for the flow problem are derived.

Section 2.4 is devoted to the transport problem. In Sections 2.4.1 – 2.4.3 we will derive a system of equations describing the transport of particles, and in Section 2.4.4 some assumptions will be introduced to obtain the final equations for the transport problem.

The coupled and decoupled measurement problems are considered in Section 2.5. Relations between the volume density of particles in the wet cell and the surface density on its active part are derived in Section 2.5.1. In Section 2.5.2 equations for the evolution of the particle density are derived, which, in combination with the flow problem, yields the mathematical model for the decoupled measurement problem. In Section 2.5.3, the influence of the particles on the fluid is modeled, and the derivation of equations for the coupled measurement problem is completed. Section 2.6 contains values of physical constants. In the appendix, some useful aids from the literature are summarized.

2.1 Notation

Both, air in the vessel and water in the wet cell (see Section 1.2), will be referred as “liquid” or “fluid”, even though air at standard conditions is gaseous. Thus we can consider liquid of fluid flow, or particle flow, or liquid-particle flow.

The bold letters $\boldsymbol{U}$ and $\boldsymbol{V}$ denote the velocity fields of the liquid and particles, respectively; p and Π denote the pressure and stress tensor, respectively. Proper densities are denoted by $\overline{\rho}$, and physical densities by ρ. For example, if $\overline{\rho_p}$ is the proper density of the particles and ϕ the volume fraction of the particles, then the physical density ρ_p is given by $\rho_p = \overline{\rho_p} \cdot \phi$.

Let Ω denote an open subset in $\mathbb{R}^N$, $N \in \{2,3\}$ (the region where the flow is considered); $\partial\Omega$ the boundary of Ω; and $\boldsymbol{\nu}$ outward directed normal unit vectors on $\partial\Omega$. The time interval where the problems are considered is denoted $I = [0,T]$, $T > 0$. If not stated differently $\boldsymbol{x}$ denotes a point in space ($\boldsymbol{x} \in \Omega$) and t a time instant ($t \in I$). It is self-evidently which physical quantities are considered as functions of $(\boldsymbol{x}, t)$. Inlet and outlet of the vessel or wet cell are assumed to be disjoint subsets of the boundary. They are denoted by Γ^{in} and Γ^{out}, respectively. The active part of the wet cell is denoted by Γ, and we assume $\Gamma \subset \partial\Omega \setminus (\Gamma^{\text{in}} \cup \Gamma^{\text{out}})$.

For two vectors $\boldsymbol{a}$, $\boldsymbol{b} \in \mathbb{R}^N$, with the components a_j, b_j, $j = 1, ..., N$, the scalar product and tensor product are

$$\boldsymbol{a} \cdot \boldsymbol{b} = \sum_{j=1}^{N} a_j\, b_j, \qquad \boldsymbol{a} \otimes \boldsymbol{b} = (a_j\, b_k)_{jk}\,, \qquad j,k = 1, ..., N,$$

and, for two matrices A, $B \in \mathbb{R}^{M \times N}$

$$A : B = \sum_{j=1}^{M} \sum_{k=1}^{N} a_{jk}\, b_{jk}.$$

For a function $\rho : \Omega \times I \to \mathbb{R}$, the gradient of ρ (the column vector) and the partial derivative with respect to time will be denoted by

$$\nabla\rho(\boldsymbol{x},t) = \frac{\partial\rho}{\partial\boldsymbol{x}}(\boldsymbol{x},t) = \left(\frac{\partial\rho}{\partial x_1}, ..., \frac{\partial\rho}{\partial x_N}\right)^T, \qquad \rho'(\boldsymbol{x},t) = \rho_t(\boldsymbol{x},t) = \frac{\partial\rho}{\partial t}(\boldsymbol{x},t),$$

and for $\boldsymbol{U} : \Omega \times I \to \mathbb{R}^N$ the gradient (Jacobi matrix) and divergence by

$$\nabla\boldsymbol{U}(\boldsymbol{x},t) = \left(\frac{\partial U_j}{\partial x_k}(\boldsymbol{x},t)\right) = \left(\frac{\partial\boldsymbol{U}}{\partial x_1}, \ldots, \frac{\partial\boldsymbol{U}}{\partial x_N}\right), \qquad \operatorname{div}\boldsymbol{U} = \sum_{j=1}^{N} \frac{\partial U_j}{\partial x_j}.$$

If Π is a tensor of the second order (a matrix), depending on $\boldsymbol{x}$ or $(\boldsymbol{x}, t)$, then the divergence $\operatorname{div}\Pi$ denotes the vector whose components are the divergences of the row vectors

$$\operatorname{div}\Pi = \left(\sum_{j=1}^{N} \frac{\partial\Pi_{1j}}{\partial x_j}, \cdots, \sum_{j=1}^{N} \frac{\partial\Pi_{Nj}}{\partial x_N}\right)^T.$$

We assume that the liquids under consideration are viscous and Newtonian, which means that the stress is related to the pressure and velocity by

$$\Pi = (-p + \lambda \operatorname{div}\boldsymbol{U})\,\mathbb{I} + \mu(\nabla\boldsymbol{U} + \nabla\boldsymbol{U}^T) \qquad \text{and} \qquad \operatorname{div}\Pi = -\nabla p + \mu\,\Delta\boldsymbol{U} + \xi\,\nabla\operatorname{div}\boldsymbol{U},$$

where μ, λ are constants depending on the liquid, $\xi = \lambda + \mu$ with μ, $\xi > 0$, see Theorem 2.B.3 and Remark 2.D.1.

2.2 Presentation of the mathematical models

First remember that we refer to the vessel shown in Figure 1.2.1.b as to the transport part of detection. The wet cell shown in Figure 1.2.1.a is associated with the measurement part of detection.

Throughout the thesis, we assume that liquids are weakly compressible. The flow of weakly compressible media is described by the following flow problem:

$$\begin{aligned} \gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0 && \text{in } \Omega \times (0,T), \\ \rho_0\, \boldsymbol{U}_t + \rho_0\, (\boldsymbol{U} \cdot \nabla)\boldsymbol{U} - \operatorname{div} \Pi &= \boldsymbol{f} && \text{in } \Omega \times (0,T), \\ \boldsymbol{U} &= \boldsymbol{U}_b && \text{on } \partial\Omega \times (0,T), \\ \boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{U}^0(\boldsymbol{x}), \qquad p(\boldsymbol{x},0) &= p^0(\boldsymbol{x}) && \text{for } t = 0. \end{aligned} \tag{2.1}$$

The theoretical investigation of (2.1) is given in Section 3.4.1.

To describe the transport part mathematically, we first derive the following system of equations:

$$\begin{aligned} \gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0, \\ \rho_0\, \boldsymbol{U}_t + \rho_0\, (\boldsymbol{U} \cdot \nabla)\boldsymbol{U} - \operatorname{div} \Pi + \alpha \,\langle \rho_p \rangle\, (\boldsymbol{U} - \langle \boldsymbol{V} \rangle) &= \boldsymbol{f}, \\ \langle \rho_p \rangle_t + \operatorname{div}\left(\langle \rho_p \rangle\, \langle \boldsymbol{V} \rangle\right) &= 0, \\ \langle \boldsymbol{V} \rangle_t + \big(\langle \boldsymbol{V} \rangle \cdot \nabla\big)\, \langle \boldsymbol{V} \rangle - \alpha\big(\boldsymbol{U} - \langle \boldsymbol{V} \rangle\big) &= 0, \end{aligned}$$

where $\langle \boldsymbol{V} \rangle$ and $\langle \rho_p \rangle$ denote the averaged velocity and density of the particle component. In order to deduce theoretical results (see Section 3.3), the equations are simplified to obtain the following initial boundary value problem:

$$\begin{aligned} \gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0 && \text{in } \Omega \times (0,T), \\ (\rho^{(0)})_t + \operatorname{div}\big(\rho^{(0)} \boldsymbol{U}^*\big) &= 0 && \text{in } \Omega \times (0,T), \\ \big(\rho_0 + \rho^{(0)}\big)\, (\boldsymbol{U}_t + (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}) - \operatorname{div} \Pi &= \boldsymbol{f} && \text{in } \Omega \times (0,T), \\ \boldsymbol{U} &= \boldsymbol{U}_b && \text{on } \partial\Omega \times (0,T), \\ \boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{U}^0(\boldsymbol{x}), \quad p(\boldsymbol{x},0) = p^0(\boldsymbol{x}), \quad \rho^{(0)}(\boldsymbol{x},0) &= \rho^0(\boldsymbol{x}) && \text{for } t = 0. \end{aligned} \tag{2.2}$$

Here $\rho^{(0)}$ denotes an approximation to the particle density $\langle \rho_p \rangle$, and we assume that $\rho^{(0)}$ satisfies the continuity equation for a smoothed velocity field $\boldsymbol{U}^* = \sigma_\delta * \boldsymbol{U}$, where σ_δ is a fixed smoothing function. During the theoretical investigation, we assume additionally that the support of ρ^0 is separated from the boundary $\partial\Omega$ by a positive distance so that, for small times, no boundary conditions for $\rho^{(0)}$ are necessary. System (2.2) is called the transport problem.

To be able to consider an operator boundary condition in the wet cell, we take the diffusion of particles into account and derive a drift-diffusion equation. Assume that the velocity field on the boundary of the wet cell $\boldsymbol{U}_b$ is known, and

$$\begin{aligned} &\boldsymbol{U}_b \cdot \boldsymbol{\nu} \le 0 && \text{on } \Gamma^{\text{in}}, \\ &\boldsymbol{U}_b \cdot \boldsymbol{\nu} \ge 0 && \text{on } \Gamma^{\text{out}}, \\ &\boldsymbol{U}_b = \boldsymbol{0} && \text{on } \partial\Omega \setminus (\Gamma^{\text{in}} \cup \Gamma^{\text{out}}). \end{aligned}$$

The following equations describe the physical processes in the wet cell:

$$
\begin{aligned}
\gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0 && \text{in } \Omega \times (0,T),\\
(\rho_p)_t + \operatorname{div}(\rho_p \boldsymbol{U}) - \beta\,\Delta\rho_p &= 0 && \text{in } \Omega \times (0,T),\\
\rho_0\, \boldsymbol{U}_t + \operatorname{div}\big(\boldsymbol{U} \otimes \big[(\rho_p + \rho_0)\boldsymbol{U} - \beta\,\nabla\rho_p\big]\big) &= \boldsymbol{f} + \operatorname{div}\Pi && \text{in } \Omega \times (0,T),\\
\boldsymbol{U} &= \boldsymbol{U}_b && \text{on } \partial\Omega \times (0,T),\\
-[\rho_p\, \boldsymbol{U}_b - \beta\,\nabla\rho_p]\cdot\boldsymbol{\nu} &= -g_p\, \boldsymbol{U}_b\cdot\boldsymbol{\nu} && \text{on } \Gamma^{\text{in}} \times (0,T),\\
-\partial_{\boldsymbol{\nu}}\rho_p &= 0 && \text{on } \partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}}),\\
-\beta\,\partial_{\boldsymbol{\nu}}\rho_p = (\eta_p)_t, \quad \eta_p &= \mathcal{A}_p(\rho_p) && \text{on } \Gamma \times (0,T),\\
\boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{U}^0(\boldsymbol{x}), \quad p(\boldsymbol{x},0) = p^0(\boldsymbol{x}), \quad \rho_p(\boldsymbol{x},0) &= \rho_p^0(\boldsymbol{x}) && \text{for } t=0 \text{ in } \Omega,\\
\eta_p(\boldsymbol{x},0) &= \eta_p^0(\boldsymbol{x}) && \text{for } t=0 \text{ on } \Gamma.
\end{aligned}
\tag{2.3}
$$

Thus, the system describes the coupled measurement problem. It is used for numerical computations in Chapter 4. In (2.3), η_p denotes the surface mass density of particles on the active part of the wet cell. The action of the active part is described by the hysteresis operator $\mathcal{A}_p$, see (2.54). In problem (2.3), the interaction between the components in both directions is accounted for. For the theoretical investigations given in Section 3.4, we have to neglect the influence of the particles on the liquid, which means that the particle density ρ_p is cancelled from the momentum balance equation. The new model-equations read:

$$
\begin{aligned}
\gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0 && \text{in } \Omega \times (0,T),\\
(\rho_p)_t + \boldsymbol{U}\cdot\nabla\rho_p - \beta\,\Delta\rho_p &= 0 && \text{in } \Omega \times (0,T),\\
\rho_0\, \boldsymbol{U}_t + \rho_0\,(\boldsymbol{U}\cdot\nabla)\,\boldsymbol{U} &= \boldsymbol{f} + \operatorname{div}\Pi && \text{in } \Omega \times (0,T),\\
\boldsymbol{U} &= \boldsymbol{U}_b && \text{on } \partial\Omega \times (0,T),\\
-[\rho_p\, \boldsymbol{U}_b - \beta\,\nabla\rho_p]\cdot\boldsymbol{\nu} &= -g_p\, \boldsymbol{U}_b\cdot\boldsymbol{\nu} && \text{on } \Gamma^{\text{in}} \times (0,T),\\
-\partial_{\boldsymbol{\nu}}\rho_p &= 0 && \text{on } \partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}}),\\
-\beta\,\partial_{\boldsymbol{\nu}}\rho_p = (\eta_p)_t, \quad \eta_p &= \mathcal{A}_p(\rho_p) && \text{on } \Gamma \times (0,T),\\
\boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{U}^0(\boldsymbol{x}), \quad p(\boldsymbol{x},0) = p^0(\boldsymbol{x}), \quad \rho_p(\boldsymbol{x},0) &= \rho_p^0(\boldsymbol{x}) && \text{for } t=0 \text{ in } \Omega,\\
\eta_p(\boldsymbol{x},0) &= \eta_p^0(\boldsymbol{x}) && \text{for } t=0 \text{ on } \Gamma.
\end{aligned}
\tag{2.4}
$$

These equations describe the decoupled measurement problem. Note that we first can find the velocity and pressure using the first and third equation, and then solve the second one for ρ_p. Thus, first compute $\boldsymbol{U}$ and then solve the problem:

$$
\begin{aligned}
\rho_t + \boldsymbol{U}\cdot\nabla\rho - \Delta\rho &= 0 && \text{in } \Omega \times (0,T),\\
\eta_t = -\partial_{\boldsymbol{\nu}}\rho, \quad \eta &= \mathcal{A}(\rho) && \text{on } \Gamma \times (0,T),\\
-\,[\rho\,\boldsymbol{U} - \nabla\rho]\cdot\boldsymbol{\nu} &= -g\,\boldsymbol{U}\cdot\boldsymbol{\nu} && \text{on } \Gamma^{\text{in}} \times (0,T),\\
-\partial_{\boldsymbol{\nu}}\rho &= 0 && \text{on } \big[\partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}})\big] \times (0,T),\\
\rho(\boldsymbol{x},0) = \rho^0(\boldsymbol{x}), \qquad \eta(\boldsymbol{x},0) &= \eta^0(\boldsymbol{x}) && \text{for } t=0.
\end{aligned}
\tag{2.5}
$$

Note that the variables are rescaled in (2.5) so that the diffusion coefficient is equal to 1, and the index p is dropped in the scaled particle density ρ and surface mass density η.

2.3 Motion of weakly compressible fluids

In this section, the continuity equation and the momentum balance equations are derived for a weakly compressible Newtonian fluid from the equations of compressible fluids. The assumption of weak compressibility will provide a relation between the density and the pressure of the fluid so that an energy equation is not needed. The derivation of the equations for compressible fluids presented here is mainly taken from the books [18, Chapter 1] and [47, Chapter 1].

The evolution of the quantities describing the motion of a viscid compressible fluid is governed by the Navier-Stokes equations

$$\begin{aligned} (\rho_f)_t + \operatorname{div}(\rho_f \boldsymbol{U}) &= 0, \\ (\rho_f \boldsymbol{U})_t + \operatorname{div}(\rho_f \boldsymbol{U} \otimes \boldsymbol{U}) + \nabla p - \mu \Delta \boldsymbol{U} - \xi \nabla \operatorname{div} \boldsymbol{U} &= \rho_f \boldsymbol{F}, \end{aligned} \tag{2.6}$$

where $\boldsymbol{U}$, ρ_f and p denote the velocity, density and pressure of the fluid, respectively. The factors μ and ξ are viscosity coefficients of the fluid, and $\boldsymbol{F}$ is the density of volume forces, e.g. gravity. The first equation in (2.6) is called continuity equation or mass conservation, and the second one represents equations of motion or momentum conservation.

Note that the product rule applied to the left-hand side of the momentum equation of (2.6) and the conservation of mass yield

$$(\rho_f \boldsymbol{U})_t + \operatorname{div}(\rho_f \boldsymbol{U} \otimes \boldsymbol{U}) = \rho_f \left[\boldsymbol{U}_t + (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}\right]. \tag{2.7}$$

In three dimensions, the system (2.6) consists of four equations for five unknown functions ρ_f, p, U_1, U_2 and U_3. Thus, an additional relation is needed in order to close the model. To this end, we assume that the fluid be weakly compressible to get a relation between ρ_f and p.

Weak compressibility means that the deviations of the density and the pressure from nominal values are small and depend linearly on each other. In this case the pressure is a function of the density only. Moreover we assume that high gradients in the pressure or velocity field and phenomena like shocks and turbulence will not occur in the vessel or wet cell. Thus, we assume that there exist reference values ρ_0 and p_0 (say the density and the pressure in the equilibrium at normal conditions) and a constant factor λ such that the linear approximation

$$\rho_f = \rho_0 + \lambda(\delta p), \qquad p = p_0 + \delta p, \qquad \text{(when } \delta p \text{ is small)} \tag{2.8}$$

reflects the physical property of the fluid. Further, we assume that all products containing δp can be neglected.

Substituting (2.8) into the source term of (2.6) yields

$$\rho_f \boldsymbol{F} \approx \rho_0 \boldsymbol{F} =: \boldsymbol{f}.$$

Inserting (2.8) into the conservation of mass for the liquid in (2.6) yields

$$\lambda (\delta p)_t + \rho_0 \operatorname{div} \boldsymbol{U} + \lambda \operatorname{div}(\delta p \, \boldsymbol{U}) = 0. \tag{2.9}$$

Denoting $\gamma := \lambda/\rho_0$ and neglecting the term containing δp, relation (2.9) can be rewritten as the following new continuity equation:

$$\gamma\, p_t + \operatorname{div} \boldsymbol{U} = 0. \tag{2.10}$$

Proceeding in the same way with the total derivative in the momentum equation of (2.6), we get

$$(\rho_f\, \boldsymbol{U})_t + \operatorname{div}\left(\rho_f\, \boldsymbol{U} \otimes \boldsymbol{U}\right) \approx \rho_0\, \boldsymbol{U}_t + \rho_0 \operatorname{div}\left(\boldsymbol{U} \otimes \boldsymbol{U}\right). \tag{2.11}$$

Note that, if (2.7) is used first, and then (2.8), the total derivative is approximated by

$$(\rho_f\, \boldsymbol{U})_t + \operatorname{div}\left(\rho_f\, \boldsymbol{U} \otimes \boldsymbol{U}\right) \approx \rho_0\, \boldsymbol{U}_t + \rho_0\ (\boldsymbol{U} \cdot \nabla)\, \boldsymbol{U}. \tag{2.12}$$

It should be stressed that no relation similar to (2.7) holds for the right-hand sides of (2.11) and (2.12). We will use (2.11) for numerical computations and (2.12) for theoretical investigations. Thus, (2.11) is used in the momentum equation in (2.3), whereas (2.12) is used in (2.1), (2.2) and (2.4). Using (2.10), products containing $\operatorname{div} \boldsymbol{U}$ can be neglected, and therefore

$$\operatorname{div}\left(\boldsymbol{U} \otimes \boldsymbol{U}\right) = (\boldsymbol{U} \cdot \nabla)\boldsymbol{U} + \boldsymbol{U} \cdot \operatorname{div} \boldsymbol{U} \approx (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}.$$

For later use in Section 2.5.3, we briefly recall the derivation of (2.6) using the same notation as in Appendix 2.A. To obtain the continuity equation consider an arbitrary control volume $V = V(t_0) \subset \overline{V} \subset \Omega_{t_0}$ at a time $t = t_0$. Set $V(t) = \boldsymbol{\phi}(V, t)$, where $\boldsymbol{\phi}$ is the mapping defined in (2.83) considered on a time interval $(t_1,\, t_2) \ni t_0$. Then, the domain $V(t)$ is formed by the same fluid particles at each time instant, therefore the mass of the element of fluid represented by the domain $V(t)$ remains constant:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V(t)} \rho_f(\boldsymbol{x}, t)\ \mathrm{d}\boldsymbol{x} = 0\ , \qquad t \in (t_1, t_2). \tag{2.13}$$

Applying the Transport Theorem 2.A.3 to (2.13) yields

$$\int_{V(t)} \left[\frac{\partial \rho_f}{\partial t}(\boldsymbol{x}, t) + \operatorname{div}\left(\rho_f\, \boldsymbol{U}\right)(\boldsymbol{x}, t)\right] \mathrm{d}\boldsymbol{x} = 0, \qquad t \in (t_1, t_2). \tag{2.14}$$

Since t is an arbitrary time instant, one can substitute $t = t_0$ and $V(t) = V(t_0) = V$ so that (2.14) holds true for arbitrary $t_0 \in (0, T)$ and arbitrary control volume V. Therefore

$$(\rho_f)_t(\boldsymbol{x}, t) + \operatorname{div}\left(\rho_f(\boldsymbol{x}, t)\, \boldsymbol{U}(\boldsymbol{x}, t)\right) = 0, \qquad t \in (0, T),\ \boldsymbol{x} \in \Omega_t,$$

which is the continuity equation in (2.6). For later purposes, rewrite the integral of the divergence in (2.14) as a surface integral

$$\int_V (\rho_f)_t\ \mathrm{d}\boldsymbol{x} = -\int_{\partial V} \rho_f\, \boldsymbol{U} \cdot \boldsymbol{\nu}\ \mathrm{d}s = -\int_{\partial V} \dot{\boldsymbol{m}} \cdot \boldsymbol{\nu}\ \mathrm{d}s, \tag{2.15}$$

where $\dot{\boldsymbol{m}} = \rho_f \boldsymbol{U}$ is the mass flux of the fluid.

The equations of motion can be derived by Newton's law of conservation of momentum in the following form: *The rate of change of the total momentum of an element of fluid formed by the same particles at each time and occupying the domain $V(t)$ at instant t is equal to the force acting on $V(t)$.*

The total momentum of fluid particles contained in $V(t)$ is given by

$$\mathcal{H}(V(t)) = \int_{V(t)} \rho_f(\boldsymbol{x},t)\,\boldsymbol{U}(\boldsymbol{x},t)\;\mathrm{d}\boldsymbol{x}. \tag{2.16}$$

Denoting by $\mathcal{F}(V(t))$ the force acting on the volume $V(t)$, the law of conservation of momentum reads

$$\frac{\mathrm{d}\mathcal{H}(V(t))}{\mathrm{d}t} = \mathcal{F}\left(V(t)\right), \qquad t \in (t_1, t_2). \tag{2.17}$$

Substituting (2.16) into (2.17), using the Transport Theorem 2.A.3, and proceeding as in the case of the continuity equation yields

$$\int_V \left[(\rho_f U_j)_t + \mathrm{div}\,(\rho_f\, U_j\, \boldsymbol{U})\right] \mathrm{d}\boldsymbol{x} = \mathcal{F}_j(V;t), \qquad j = 1,2,3, \tag{2.18}$$

for the j-th component of the momentum, arbitrary $t \in (0,T)$ and arbitrary control volume V, where the components of $\mathcal{F}(V;t)$ are denoted by $\mathcal{F}_j(V;t)$.

Here only the volume force (also called the outer or body force) and the surface force (inner force) exerted by the fluid contained outside the domain V on its boundary are considered. Denoting the density of the volume force by $\boldsymbol{F} \in [\mathcal{C}^1(\mathcal{M})]^3$ and expressing the surface force using the stress tensor $\Pi = (\Pi_{ij})_{i,j=1}^3$ that characterizes the density and direction of the surface force, the forces acting on V are given by

$$\mathcal{F}(V;t) = \int_V \rho_f(\boldsymbol{x},t)\boldsymbol{F}(\boldsymbol{x},t)\;\mathrm{d}\boldsymbol{x} + \int_{\partial V} \Pi \cdot \boldsymbol{\nu}\;\mathrm{d}s. \tag{2.19}$$

Substituting (2.19) into (2.18), using Green's Theorem, and taking into account that t and V are arbitrary yields

$$\frac{\partial}{\partial t}\big(\rho_f\, U_j\big)_t + \frac{\partial}{\partial x_k}\big(\rho_f\, U_j\, U_k\big) = \rho_f\, F_j + \frac{\partial\, \Pi_{jk}}{\partial x_k}, \qquad j = 1,2,3,$$

for j-th component of the momentum equation (summation over repeated indexes is assumed). Or in tensor notation

$$(\rho_f\, \boldsymbol{U})_t + \mathrm{div}\,(\rho_f\, \boldsymbol{U} \otimes \boldsymbol{U}) = \rho_f\, \boldsymbol{F} + \mathrm{div}\,\Pi \tag{2.20}$$

Assuming that the fluid is Newtonian and using Stokes' Postulates given in Section 2.B yields that the tensor Π is given by Theorem 2.B.1:

$$\Pi = (-p + \lambda\,\mathrm{div}\,\boldsymbol{U})\,\mathbb{I} + 2\,\mu\,\mathbb{D}. \tag{2.21}$$

If the relations $\mu \geq 0$, $3\lambda + 2\mu = 0$ hold (see [18]), we get

$$\mathrm{div}\,\Pi = -\nabla p + \mu\Delta\boldsymbol{U} + \xi\,\nabla\mathrm{div}\,\boldsymbol{U}, \qquad \xi = \mu + \lambda \geq 0. \tag{2.22}$$

Substituting (2.22) into (2.20) yields the momentum equation claimed in (2.6). Further note that (2.20) can written as

$$\rho_f\, \boldsymbol{U}_t + (\dot{\boldsymbol{m}} \cdot \nabla)\boldsymbol{U} = \mathrm{div}\,\Pi + \rho_f\, \boldsymbol{F}. \tag{2.23}$$

2.4 Transport of particles

In this section we derive the equations for the transport problem. The chamber, where the transport phenomena occur, is schematically shown in Figure 2.4.1 in two dimensions. The arrows indicate the flow direction of inflow and outflow of the liquid.

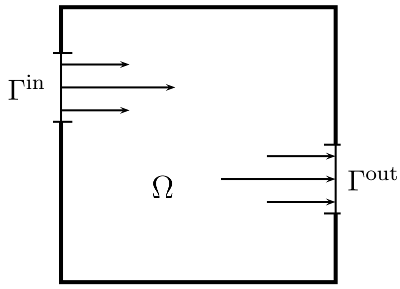


Figure 2.4.1: Scheme of the vessel

Under the assumption that the velocity field $\boldsymbol{U}$ of the liquid is known, we derive equations of motion for the particles as follows:

$$\rho_p \,\mathrm{d}\boldsymbol{V} = \alpha \,\rho_p \,(\boldsymbol{U} - \boldsymbol{V})\,\mathrm{d}t + \beta \sqrt{\rho_p}\,\mathrm{d}\boldsymbol{W}_t, \tag{2.24}$$

where ρ_p and $\boldsymbol{V}$ denote the particle density and the bulk velocity of the particles, respectively, and α and β are constants determined by properties of the liquid and the particles. The right-hand side of (2.24) describes the momentum transfer from the liquid to the particles. Since the momentum has to be conserved, the momentum transfer from the particles to the liquid has to be considered too. This will be achieved by subtracting the term

$$\alpha \,\langle\rho_p\rangle\,(\boldsymbol{U} - \langle\boldsymbol{V}\rangle)$$

from the right-hand side of the momentum equation of the liquid. In order to close the model, results from the Boltzmann equation will be used to obtain the continuity equation for the particles.

2.4.1 Motion of a single particle

The context of this section is based on [64]. The motion of a single particle transported by a fluid is given by

$$\frac{\mathrm{d}\boldsymbol{V}_p}{\mathrm{d}t} = \boldsymbol{F}_{\text{drag}} + \boldsymbol{F}_{\text{bi}}\,, \qquad \frac{\mathrm{d}\boldsymbol{x}_p}{\mathrm{d}t} = \boldsymbol{V}_p. \tag{2.25}$$

Here $\boldsymbol{V}_p$ denotes the particle velocity, and $\boldsymbol{x}_p$ the position. The force causing the acceleration of the particle is split into the macroscopic drag force $\boldsymbol{F}_{\text{drag}}$ and the Brownian force $\boldsymbol{F}_{\text{bi}}$ arising from the molecular motion. Since the particle is larger than a molecule of the fluid, the drag force is given by Stokes' formula

$$\boldsymbol{F}_{\text{drag}} = \frac{3\pi\,\mu\,d_p(\boldsymbol{U} - \boldsymbol{V}_p)}{m_p\,C_c},$$

where d_p, m_p and $\boldsymbol{V}_p$ are the diameter, mass, and velocity of the particle, respectively, and μ and $\boldsymbol{U}$ are the dynamical viscosity and velocity of the fluid, respectively; C_c denotes the Cunningham slip correction (see formula (2.82)).

The fluctuations are given by Gaussian random variables with

$$\langle \boldsymbol{F}_{\mathrm{bi}}(t) \rangle = 0\,, \qquad \langle \boldsymbol{F}_{\mathrm{bi}}(t) \cdot \boldsymbol{F}_{\mathrm{bi}}(t') \rangle = \frac{2\,k\,\theta\,f\,\delta(t'-t)}{m_p^2}.$$

Here k denotes Boltzmann's constant, θ the temperature, and f the friction coefficient (see [21]) given by

$$f = \frac{3\,\pi\,\mu\,d_p}{C_c}.$$

In the following, we will assume that C_c is constant. As in [37, 64] the components of the Brownian force can be written as

$$F^i_{\mathrm{bi}} = G^i \sqrt{\frac{\pi\,S_0}{\Delta t}}, \qquad \text{where} \qquad S_0 = \frac{216\,\nu\,k\,\theta}{\pi^2\,\rho_f\,d_p^5\,(\overline{\rho_p}/\overline{\rho_f})^2\,C_c}. \tag{2.26}$$

In (2.26), G^i is a Gaussian random variable, ν the kinematic viscosity of the fluid related to the dynamic viscosity as $\mu = \rho_f\,\nu$. Introducing the abbreviations

$$\alpha := \frac{3\pi\,\mu\,d_p}{m_p\,C_c}\,, \qquad \beta_* := \sqrt{\pi\,S_0} = \sqrt{\frac{216\,\mu\,k\,\theta}{\pi\,d_p^5\,\rho_p^2\,C_c}} \tag{2.27}$$

and letting $\Delta t \to 0$, equations (2.25) become the Langevin equations from the Ornstein-Uhlenbeck theory of Brownian particles (see [61, 45]).

$$\begin{aligned} \mathrm{d}\boldsymbol{x}_p &= \boldsymbol{V}_p\,\mathrm{d}t, \\ \mathrm{d}\boldsymbol{V}_p &= \alpha\,(\boldsymbol{U} - \boldsymbol{V}_p)\,\mathrm{d}t + \beta_*\,\mathrm{d}\boldsymbol{W}_t. \end{aligned} \tag{2.28}$$

2.4.2 Averaged motion of particles

In Section 2.4.1, the influence of the liquid on a particle is model by the Gaussian random process $\mathrm{d}\boldsymbol{W}_t$. To derive relations for the bulk density and the bulk velocity of the particles, we use that the arithmetic mean value of independently normally distributed random variables is again normally distributed. More precisely, if $G_1, ..., G_n,\ n \in \mathbb{N}$ are normally distributed with $G_j \sim \mathcal{N}(\mu_j, \sigma_j^2)$, then the arithmetic mean value S_n is normally distributed:

$$S_n = \frac{1}{n}\sum_{j=1}^{n} G_j \sim \mathcal{N}\left(\mu_S,\,\sigma_S^2\right) \qquad \text{where} \qquad \mu_S = \frac{1}{n}\sum_{j=1}^{n}\mu_j\,, \quad \sigma_S^2 = \frac{1}{n^2}\sum_{j=1}^{n}\sigma_j^2. \tag{2.29}$$

Definition 2.4.1. *For a point $\boldsymbol{x} \in \mathbb{R}^N$, consider a small neighbourhood V of $\boldsymbol{x}$. Define the* bulk density *ρ_p of particles at $\boldsymbol{x}$ at time t as the ratio of the total mass of the particles contained in V divided by the volume of V. If V contains n particles of equal mass m_p, one can write*

$$\rho_p(\boldsymbol{x}, t) = \frac{1}{|V|}\sum_{\boldsymbol{x}_k(t)\in V} m_p = \frac{m_p\,n}{|V|},$$

where $\boldsymbol{x}_k(t)$ denotes the position of the particle k at time t. In a similar way, the bulk velocity $\boldsymbol{V}$ *is defined as the mean value of the velocities of the particles contained in V:*

$$\boldsymbol{V}(\boldsymbol{x},t) = \begin{cases} \frac{1}{n} \sum\limits_{\boldsymbol{x}_k(t)\in V} \boldsymbol{V}_{p,k}(\boldsymbol{x}_k(t),t) = \frac{m_p}{\rho_p(\boldsymbol{x},t)|V|} \sum\limits_{\boldsymbol{x}_k(t)\in V} \boldsymbol{V}_{p,k}(\boldsymbol{x}_k(t),t) & \textit{if } n \geq 1, \\ \boldsymbol{0} & \textit{else.} \end{cases}$$

To derive an equation for the bulk velocity $\boldsymbol{V}$, the differential $\mathrm{d}t$ is replaced by a finite time interval Δt and $\mathrm{d}\boldsymbol{W}_t$ is replaced by $G_k\sqrt{\Delta t}$ for particle k, where $G_k \sim \mathcal{N}(0,1)$ is the Gaussian probability variable (see (2.26). Averaging (2.28) over all particles in V and using Definition 2.4.1 yields

$$\begin{aligned} \Delta \boldsymbol{x} &= \boldsymbol{V}(\boldsymbol{x}(t),t)\Delta t \\ \Delta \boldsymbol{V} &= \frac{\alpha}{n} \sum_{\boldsymbol{x}_k(t)\in V} (\boldsymbol{U} - \boldsymbol{V}_{p,k})\ \Delta t + \frac{\beta_* \sqrt{\Delta t}}{n} \sum_{\boldsymbol{x}_k(t)\in V} G_k. \end{aligned} \tag{2.30}$$

If the drift velocity $\boldsymbol{U}$ is assumed to be continuous, the mean value of $\boldsymbol{U}$ can be approximated by $\boldsymbol{U}(\boldsymbol{x},t)$. Using (2.29) and Definition 2.4.1, the stochastic term can be rewritten as

$$\frac{1}{n} \sum_{\boldsymbol{x}_k(t)\in V} G_k = n^{-1/2}\, G = \left(\frac{m_p}{\rho_p\,|V|}\right)^{1/2} G, \qquad G \sim \mathcal{N}(0,1). \tag{2.31}$$

Inserting (2.31) into (2.30) yields, for the region where $\rho_p > 0$,

$$\Delta \boldsymbol{V} = \alpha\,(\boldsymbol{U} - \boldsymbol{V})\ \Delta t + \frac{\beta}{\sqrt{\rho_p}}\, G\sqrt{\Delta t}, \qquad \text{where} \qquad \beta = \beta_* \left(\frac{m_p}{|V|}\right)^{1/2}. \tag{2.32}$$

Let $\rho_{\min} = m_p/|V|$ be interpreted as the minimal particle density, i.e. $\rho_p = 0$ if V contains no particles, or $\rho_p \geq \rho_{\min}$ if V contains at least one particle. In the case of integer numbers of particles ($n \in \{1,\ 2\ldots\}$) it holds

$$0 \leq \frac{\beta}{\sqrt{\rho_p}} = \frac{\beta_*}{\sqrt{n}} \leq \beta_*.$$

For $\Delta t \to 0$, replace $G\sqrt{\mathrm{d}t}$ by $\mathrm{d}\boldsymbol{W}_t$, and (2.30) becomes

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} &= \boldsymbol{V}(\boldsymbol{x}(t),t), \\ \mathrm{d}\boldsymbol{V}(\boldsymbol{x}(t),t) &= \alpha\ (\boldsymbol{U}(\boldsymbol{x}(t),t) - \boldsymbol{V}(\boldsymbol{x}(t),t))\ \mathrm{d}t + \frac{\beta}{\sqrt{\rho_p}}\ \mathrm{d}\boldsymbol{W}_t. \end{aligned} \tag{2.33}$$

Multiplying the second equation by ρ_p, we get the conservation of momentum (2.24).

In order to describe the transport of particles through the vessel, we are not interested in the description of the motion of single particles, and therefore, not in the evolution of the stochastic quantities $\boldsymbol{V}$ and ρ_p. Our goal is to describe the evolution of the expected values of the particle velocity and density, i.e. $\langle \boldsymbol{V} \rangle$ and $\langle \rho_p \rangle$.

To compute the expectation of the both sides of (2.24), the stochastic differential $\mathrm{d}\boldsymbol{W}_t$ is understood in the Ito sense. Therefore, the probabilistic part $\mathrm{d}\boldsymbol{W}_t$ in (2.24) does not influence

ρ_p and $\boldsymbol{V}$ until time instant $t + \mathrm{d}t$. Since the Brownian motion has independent increments, and because we assume that the particles are dilute enough so that the Brownian force is generated by the liquid only, we obtain that $\rho_p^{\pm 1/2}$ and $\mathrm{d}\boldsymbol{W}_t$ are stochastically independent at each time instant. This argument is more clear, if the time discrete equations (2.30) and (2.32) are considered. The random variables G, G_k, at time t are assumed to be independent from that at preceding time instances, and therefore the variables G, G_k, $\boldsymbol{V}$ and ρ_p are independent because $\boldsymbol{V}$ and ρ_p at time t are generated by G and G_k occurring at preceding time instances. Moreover, if the particles are rarefied the collisions of a certain particle with liquid molecules do not influence the collisions of an other particle with liquid molecules. Therefore, it is natural to assume that $\rho_p^{\pm 1/2}$ and G are independent in (2.32).

Thus, computing the expectation of the both sides of the second equation in (2.33) yields the evolution of $\langle \boldsymbol{V} \rangle$:

$$\mathrm{d}\langle \boldsymbol{V} \rangle = \alpha\,(\boldsymbol{U} - \langle \boldsymbol{V} \rangle)\,\mathrm{d}t. \tag{2.34}$$

To obtain an equation for the momentum, multiply (2.34) by $\langle \rho_p \rangle$ to get

$$\langle \rho_p \rangle \, \frac{\mathrm{d}\,\langle \boldsymbol{V} \rangle}{\mathrm{d}t} = \langle \rho_p \rangle \; \alpha\,(\boldsymbol{U} - \langle \boldsymbol{V} \rangle)\,. \tag{2.35}$$

Thus, the expected momentum transfer from the liquid to the particles at time t is $\langle \rho_p \rangle \; \alpha \; (\boldsymbol{U} - \langle \boldsymbol{V} \rangle)$.

We complete this section by combining systems (2.6) and (2.35) and using the weak compressibility of the liquid to obtain

$$\begin{aligned} \gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0, \\ \rho_0\, \boldsymbol{U}_t + \rho_0\, (\boldsymbol{U}\cdot\nabla)\boldsymbol{U} - \operatorname{div} \Pi^{(l)} &= \boldsymbol{f}, \\ \langle \rho_p \rangle \, \frac{\mathrm{d}\,\langle \boldsymbol{V} \rangle}{\mathrm{d}t} - \langle \rho_p \rangle \; \alpha\,(\boldsymbol{U} - \langle \boldsymbol{V} \rangle) &= \boldsymbol{0}. \end{aligned} \tag{2.36}$$

In N space dimensions, this is a system of $2N + 1$ equations for $2N + 2$ unknowns U_1, $\langle V \rangle_1$, ..., U_N, $\langle V \rangle_N$, p and $\langle \rho_p \rangle$. Thus, a continuity equation for $\langle \rho_p \rangle$ is needed. Moreover, (2.36) contains no term that describes the influence of the particles on the liquid. These aspects are considered in Section 2.4.3. We do not cancel the factor $\langle \rho_p \rangle$ in (2.36) to keep the corresponding equation being the momentum conservation law of the particles. This will be useful in Sections 2.4.3 and 2.4.4.

2.4.3 Interaction with the liquid

The system we are considering consists of two phases, the liquid and particle phases. Comparing the momentum equations for the fluid in (2.6) and for the particles in (2.24), we see that the liquid transfers momentum to the particles, but there is no term describing the influence of the particles on the liquid. However, the momentum has to be conserved and therefore, the amount of the momentum transfered to the particles has to be subtracted from the momentum of the liquid. Moreover, as it is mentioned at the end of Section 2.4.2, the continuity equation for $\langle \rho_p \rangle$ is necessary.

The following arguments are taken from [11, 12, 62]. The desired equation will be obtained using the results of Section 2.D applied to a Boltzmann gas consisting of two species: the liquid labeled by 1 and the particles labeled by 2. In the similar way, we obtain a term that describes the momentum transfer from the liquid to the particles. Let us assume the following assumptions.

1. The average $\langle\cdot\rangle$ over the Brownian motion and the average $\int[\cdot]\mathrm{d}\boldsymbol{\xi}$ over the microscopic velocity yield the same result. Using the notation of Section 2.D, this implies

$$\begin{aligned} \boldsymbol{v}^{(1)} &= \boldsymbol{U}, & \rho_l &= \rho^{(1)}, \\ \boldsymbol{v}^{(2)} &= \langle \boldsymbol{V} \rangle, & \langle \rho_p \rangle &= \rho^{(2)}, \end{aligned} \tag{2.37}$$

2. The tensor $\Pi^{(1)}$ is given in terms of $p^{(1)}$ and $\boldsymbol{v}^{(1)}$ by formula (2.21). The tensor $\Pi^{(2)}$ is equal to zero because the particle continuum does not have any internal pressure or stress.

Application of the results of Section 2.D. The evolution of a mixture of two species can be described in terms of their one-particle distributions. Denote by f_1 and f_2 the one-particle distributions of the liquid and particles, respectively. Then $f_j(\boldsymbol{x}, \boldsymbol{\xi}, t)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{\xi}$ is the expected mass of molecules of species j which, at time t, have positions lying within a volume element $\mathrm{d}\boldsymbol{x}$ about $\boldsymbol{x}$ and velocities lying within a momentum-space element $\mathrm{d}\boldsymbol{\xi}$ about $\boldsymbol{\xi}$. Therefore,

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f_j(\boldsymbol{x}, \boldsymbol{\xi}, t)\,\mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{x} = M_j, \qquad j = 1, 2,$$

where M_1 and M_2 are the total masses of the liquid and the particles, respectively.

The one-particle functions satisfy the Boltzmann equations (2.91) for $n = 2$:

$$\begin{aligned} \frac{\partial f_1}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f_1}{\partial \boldsymbol{x}} &= Q_{11}(f_1, f_1) + Q_{12}(f_1, f_2), \\ \frac{\partial f_2}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f_2}{\partial \boldsymbol{x}} &= Q_{21}(f_2, f_1) + Q_{22}(f_2, f_2), \end{aligned}$$

where the macroscopic force is neglected. The collision terms $Q_{jk}(f_j, f_k)$ describe the influence of collisions between particles of species j and k on the evolution of the one-particle function of species j. If f_1 and f_2 are known, the macroscopic quantities describing the flow are given by

$$\rho^{(j)} = \int_{\mathbb{R}^N} f_j\,\mathrm{d}\boldsymbol{\xi}, \qquad (\rho\boldsymbol{v})^{(j)} = \int_{\mathbb{R}^N} \boldsymbol{\xi} f_j\,\mathrm{d}\boldsymbol{\xi}, \qquad \boldsymbol{v}^{(j)} = \frac{(\rho\boldsymbol{v})^{(j)}}{\rho^{(j)}},$$

where $\rho^{(j)}$, $(\rho\boldsymbol{v})^{(j)}$ and $\boldsymbol{v}^{(j)}$ denote the mass density, momentum, and mass velocity of species j, respectively.

By (2.93) the macroscopic variables satisfy the continuity equations for each phase:

$$\left(\rho^{(j)}\right)_t + \operatorname{div}\left(\rho^{(j)}\,\boldsymbol{v}^{(j)}\right) = 0, \qquad j = 1, 2, \tag{2.38}$$

and the conservation of the total momentum reads

$$\sum_{j=1}^{2}\left[\left(\rho^{(j)}\boldsymbol{v}^{(j)}\right)_t + \operatorname{div}\left(\rho^{(j)}\boldsymbol{v}^{(j)}\otimes\boldsymbol{v}^{(j)} + \Pi^{(j)}\right)\right] = \boldsymbol{0}. \tag{2.39}$$

The components of the tensor $\Pi^{(j)}$ are given by

$$\Pi_{ik}^{(j)} = \int_{\mathbb{R}^N} c_i^{(j)}\,c_k^{(j)}\,f_j\,\mathrm{d}\boldsymbol{\xi},$$

where $\boldsymbol{c}^{(j)} = \boldsymbol{\xi} - \boldsymbol{v}^{(j)}$ is the peculiar velocity of the j-th species. Using the mass conservations (2.38), equation (2.39) can be rewritten as

$$\sum_{j=1}^{2} \left[\rho^{(j)} \frac{\mathrm{d}\boldsymbol{v}^{(j)}}{\mathrm{d}t} + \operatorname{div} \Pi^{(j)} \right] = \mathbf{0}. \tag{2.40}$$

Random forces. In contrast to the above derivation, equation (2.25) defines a probabilistic model for the evolution of the particles (component 2). Using the same notation as for the Boltzmann equation, we write

$$\mathrm{d}\boldsymbol{\xi} = \boldsymbol{F}(t, \boldsymbol{x}, \boldsymbol{\xi})\,\mathrm{d}t, \qquad \text{with } \boldsymbol{F}\,\mathrm{d}t = \alpha(\boldsymbol{U} - \boldsymbol{\xi})\,\mathrm{d}t + \beta\,\mathrm{d}\boldsymbol{W}_t \tag{2.41}$$

and assume that the force acting on the particles comes from the liquid only. In other words, there are no collisions of particles with each other. Then, one can show that the distribution function f_2 of the particles satisfies the Fokker-Planck equation (see [11, II.9])

$$\frac{\partial f_2}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f_2}{\partial \boldsymbol{x}} = \frac{\beta}{2} \Delta_{\boldsymbol{\xi}} f_2 - \frac{\partial}{\partial \boldsymbol{\xi}} \left[\alpha(\boldsymbol{U} - \boldsymbol{\xi}) f_2 \right], \tag{2.42}$$

where $\Delta_{\boldsymbol{\xi}}$ denotes the Laplacian with respect to the components of $\boldsymbol{\xi}$.

We postulate now that the above described approach related to collisions and the probabilistic approach described by (2.25), (2.41) and (2.42) yield the same result. Therefore, the continuity equation for the particles can be used. To get the conservation of momentum, multiply (2.42) by $\boldsymbol{\xi}$, integrate over $\mathbb{R}^N$, and use the conservation of mass to obtain:

$$\begin{aligned} \rho^{(2)} \frac{\mathrm{d}\boldsymbol{v}^{(2)}}{\mathrm{d}t} + \operatorname{div}\Pi^{(2)} &= \int_{\mathbb{R}^N} \left[\frac{\beta}{2} \boldsymbol{\xi}\, \Delta_{\boldsymbol{\xi}} f_2 + \alpha(\boldsymbol{U} - \boldsymbol{\xi}) f_2 \right] \mathrm{d}\boldsymbol{\xi} \\ &= \alpha \rho^{(2)} \big(\boldsymbol{U} - \boldsymbol{v}^{(2)} \big) + \frac{\beta}{2} \int_{\mathbb{R}^N} \boldsymbol{\xi}\, \Delta_{\boldsymbol{\xi}} f_2 \mathrm{d}\boldsymbol{\xi}. \end{aligned} \tag{2.43}$$

Combining both approaches. Equations (2.43) and (2.35) yield

$$\rho^{(2)} \frac{\mathrm{d}\boldsymbol{v}^{(2)}}{\mathrm{d}t} = \alpha \rho^{(2)} \big(\boldsymbol{v}^{(1)} - \boldsymbol{v}^{(2)} \big), \qquad \frac{\beta}{2} \int_{\mathbb{R}^N} \left[\boldsymbol{\xi}\, \Delta_{\boldsymbol{\xi}} f \right] \mathrm{d}\boldsymbol{\xi} = \operatorname{div}\Pi^{(2)} = 0. \tag{2.44}$$

Substituting (2.37) and (2.44) into (2.40) and inserting the macroscopic force again denoted by $\boldsymbol{F}$ yield the conservation for the liquid

$$\rho_l\, \boldsymbol{U}_t + \rho_l \left(\boldsymbol{U} \cdot \nabla \right) \boldsymbol{U} - \operatorname{div} \Pi^{(1)} = \rho_l \boldsymbol{F} - \alpha \left\langle \rho_p \right\rangle \left(\boldsymbol{U} - \langle \boldsymbol{V} \rangle \right). \tag{2.45}$$

Finally, combining equation (2.34), continuity equations (2.38), momentum equation (2.45), and using the weak compressibility of the liquid, we get

$$\begin{aligned} \gamma p_t + \operatorname{div} \boldsymbol{U} &= 0, \\ \rho_0\, \boldsymbol{U}_t + \rho_0 \left(\boldsymbol{U} \cdot \nabla \right) \boldsymbol{U} - \operatorname{div} \Pi + \alpha \left\langle \rho_p \right\rangle \left(\boldsymbol{U} - \langle \boldsymbol{V} \rangle \right) &= \boldsymbol{f}, \\ \left\langle \rho_p \right\rangle_t + \operatorname{div} \left(\left\langle \rho_p \right\rangle \langle \boldsymbol{V} \rangle \right) &= 0, \\ \langle \boldsymbol{V} \rangle_t + \big(\langle \boldsymbol{V} \rangle \cdot \nabla \big) \langle \boldsymbol{V} \rangle - \alpha \big(\boldsymbol{U} - \langle \boldsymbol{V} \rangle \big) &= 0. \end{aligned} \tag{2.46}$$

In system (2.46) the number of equations equals to the number of unknowns ($2N + 2$). Therefore, one can hope that the solvability under suitable initial and boundary conditions can be proved. Nevertheless, in Section 2.4.4, we will introduce further simplifications to ensure the applicability of the method used in Section 3.3 will work.

2.4.4 A simplified model for the particle transport

In order to derive a model for which we can show the existence and uniqueness of weak solutions, the system (2.46) has to be simplified. To this end, $\langle \boldsymbol{V} \rangle$ and $\langle \rho_p \rangle$ are expanded in the small parameter α^{-1} so that the momentum conservation for the particles is not necessary anymore. In this section, the following model is derived

$$\begin{aligned} \gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0, \\ \big(\rho^{(0)}\big)_t + \operatorname{div}\big(\rho^{(0)} \boldsymbol{U}^*\big) &= 0, \\ \big(\rho_0 + \rho^{(0)}\big)\big(\boldsymbol{U}_t + (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}\big) + \nabla p - \mu \Delta \boldsymbol{U} - \xi \nabla \operatorname{div} \boldsymbol{U} &= \boldsymbol{f}, \end{aligned} \tag{2.47}$$

where $\boldsymbol{U}^* = \boldsymbol{U} * \sigma_\delta$ with a fixed smoothing function σ_δ and $\rho^{(0)}$ denotes the expansion term of $\langle \rho_p \rangle$ of order 0. System (2.47) will be derived from (2.46) under the following assumptions.

1. The average density $\langle \rho_p \rangle$ and the average particle velocity $\langle \boldsymbol{V} \rangle$ can be expanded in the small parameter $\epsilon = \alpha^{-1}$, that is

$$\begin{aligned} \langle \rho_p \rangle &= \rho^{(0)} & &(+\epsilon \rho^{(1)} + \epsilon^2 \rho^{(2)} + ...), \\ \langle \boldsymbol{V} \rangle &= \boldsymbol{V}^{(0)} + \epsilon \boldsymbol{V}^{(1)} & &(+\epsilon^2 \boldsymbol{V}^{(2)} + ...). \end{aligned} \tag{2.48}$$

2. The approximation $\rho^{(0)}$ of $\langle \rho_p \rangle$ of order 0 fulfills the continuity equation with the smoothed velocity-field, that is

$$(\rho^{(0)})_t + \operatorname{div}\big(\rho^{(0)} \boldsymbol{U}^*\big) = 0.$$

To justify the first assumption consider Table 2.6.4. From the values of α for $\mathrm{Ti\,O_2}$ particles of the diameter less than $1\mu\mathrm{m}$ in air or water, we see that $\epsilon < 5 \cdot 10^{-5}$ in the both media. The second assumption is explained in the beginning of the chapter.

Substituting the expansion (2.48) into (2.34) yields

$$\epsilon \frac{\mathrm{d}\boldsymbol{V}^{(0)}}{\mathrm{d}t} + \epsilon^2 \frac{\mathrm{d}\boldsymbol{V}^{(1)}}{\mathrm{d}t} + ... = \Big(\boldsymbol{U} - \boldsymbol{V}^{(0)} - \epsilon \boldsymbol{V}^{(1)} - ...\Big).$$

Comparing the coefficients yields

$$\begin{aligned} \epsilon^0 : &\quad \boldsymbol{V}^{(0)} = \boldsymbol{U}, \\ \epsilon^1 : &\quad \boldsymbol{V}^{(1)} = -\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -\left[\boldsymbol{U}_t + (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}\right]. \end{aligned} \tag{2.49}$$

Inserting (2.48) into (2.45) and using (2.49), we get

$$\begin{aligned} &\rho_l\, \boldsymbol{U}_t + \rho_l\, (\boldsymbol{U} \cdot \nabla)\, \boldsymbol{U} - \operatorname{div} \Pi - \rho_l \boldsymbol{F} \\ &= \alpha \Big(\rho^{(0)} + \epsilon^1 \rho^{(1)} + ...\Big) \Big(-\epsilon^1 \frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} + \epsilon^2\, \boldsymbol{V}^{(2)} + ...\Big) \\ &= -\rho^{(0)}\big(\boldsymbol{U}_t + (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}\big) + ..., \end{aligned} \tag{2.50}$$

since the only term appearing with ϵ^0 is $\rho^{(0)} \boldsymbol{V}^{(1)}$. For a weakly compressible fluid, (2.50) is identical to the conservation of the total momentum in (2.47).

To obtain an equation for $\rho^{(0)}$ substitute the expansion (2.48) into the mass conservation for the particle phase in (2.46) to obtain:

$$0 = \epsilon^0 \left[\rho_t^{(0)} + \operatorname{div}\big(\rho^{(0)}\boldsymbol{U}\big)\right] + \epsilon^1 \left[\rho_t^{(1)} + \operatorname{div}\left(\rho^{(0)}\boldsymbol{V}^{(1)} + \rho^{(1)}\boldsymbol{U}\right)\right] + \epsilon^2 ... ,$$

and for ϵ^0:

$$(\rho^{(0)})_t + \operatorname{div}\big(\rho^{(0)}\,\boldsymbol{U}\big) = 0.$$

By the second assumption, $\boldsymbol{U}$ can be replaced by $\boldsymbol{U}^*$ which yields the mass conservation equation of particles of (2.47).

2.5 Measurement of particles

In this section, the equations for the description of the measurement part (see Figure 1.2.1.a, page 3) are derived. The model of the wet cell is the same as in [8] and [4].

This section is structured as follows. The description of the active part of the wet cell is given in Section 2.5.1. This shows why the systems (2.2) or (2.46) are not used to describe the measurement part. The evolution of the particles density in the interior of the wet cell is considered in Section 2.5.2, and the equations for the coupled measurement problem are derived in Section 2.5.3. This model equations are used for numerical computations in Chapter 4.

2.5.1 Mathematical description of the active part of the wet cell

Denote the interior of the wet cell by Ω, the whole boundary by $\partial\Omega$, and the outward directed unit normal on $\partial\Omega$ by $\boldsymbol{\nu}$. The inlet, outlet, and active part denoted by $\Gamma^{\text{in}}, \Gamma^{\text{out}}$ and Γ, respectively, are mutually disjoint subsets of $\partial\Omega$. We suppose for simplicity that Ω is the cube $(0,1)^N$, and Γ is contained in the plane $\{x_N = 0\}$. Then $\boldsymbol{\nu} = -\boldsymbol{e}_N$ on Γ, where $\boldsymbol{e}_N$ is the unit vector along the x_N-axis.

Assume that the particles adhered to the aptamers are located in the region

$$\Gamma_\delta := \left\{\boldsymbol{x} \in \mathbb{R}^N \;:\; (x_1, ..., x_{N-1}, 0)^T \in \Gamma \;\wedge\; -\delta \le x_N \le 0\right\}$$

By our hypothesis, the particles entering Γ_δ are instantaneously immobilized and trapped. Let ϕ be the volume fraction of particles in Ω; $\overline{\phi}$ the volume fraction of the particles in Γ_δ, and $\overline{\phi}_{\max}$ the maximal value of $\overline{\phi}$. Denote the proper density of the particles by $\overline{\rho_p}$, then the mass η_p of trapped particles per surface unit of Γ is given by

$$\eta_p(\boldsymbol{x}) = \overline{\rho_p} \int_0^\delta \overline{\phi}\,(\boldsymbol{x} + r\,\boldsymbol{\nu})\;\mathrm{d}r.$$

Denote the mass flux of the particles by $\dot{\boldsymbol{m}}_p$, then the mass conservation law reads

$$(\eta_p)_t = \dot{\boldsymbol{m}}_p \cdot \boldsymbol{\nu}, \qquad \text{on } \Gamma. \tag{2.51}$$

In order to close the model, a relation between η_p and ρ_p or between $\bar{\phi}$ and ϕ has to be specified, which plays the role of a constitutive relation that accounts for the adhesion properties of the aptamer. First, the adhered particles are not released any more. Therefore, η_p and $\bar{\phi}$ should be monotonically increasing. Second, there exist two thresholds ϕ_0 and ϕ_1 such that the aptamer can not bind particles, if either $\phi|_\Gamma \le \phi_0$ (insufficient concentration for the activation), or $\phi|_\Gamma \ge \phi_1$ (exhaustion of free aptameres). Since the particles arriving at Γ are immediately absorbed until saturation and not detached, define the hysteresis operator $\mathcal{A}_\phi$ by

$$\mathcal{A}_\phi(\xi)(t) = \operatorname{ess\,sup}\left\{H_\phi\left(\xi(\tau)\right) \,:\, \tau \le t\right\}, \qquad \text{for } \xi \in L^\infty(0,T), \tag{2.52}$$

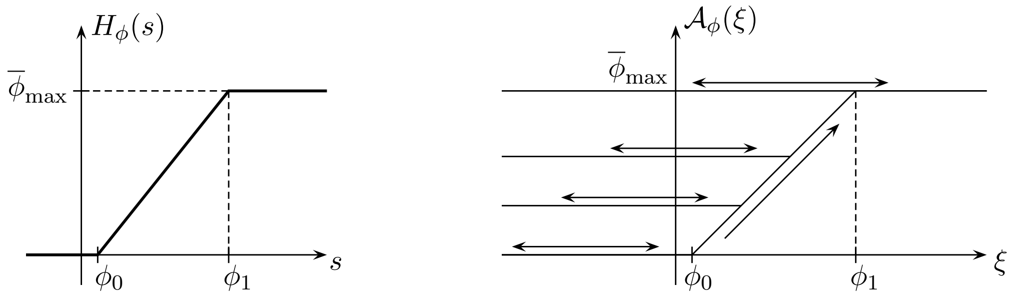
where

$$H_\phi(s) = \begin{cases} 0 & \text{if } s < \phi_0, \\ a(s-\phi_0) & \text{if } s \in [\phi_0, \phi_1], \\ \bar{\phi}_{\max} & \text{if } s > \phi_1, \end{cases}$$

and $a = \overline{\phi}_{\max}/(\phi_1 - \phi_0)$. Then the constitutive relation between $\overline{\phi}$ and ϕ reads

$$\overline{\phi}(\boldsymbol{x}, t) = \mathcal{A}_\phi\left(\phi(\boldsymbol{x}, \cdot)\right)(t), \qquad \boldsymbol{x} \in \Gamma,\, t \in (0,T). \tag{2.53}$$

See Figure 2.5.2 for an illustration.



2.5.2.a: Graph of H_ϕ 2.5.2.b: Action of the hysteresis operator $\mathcal{A}_\phi$

Figure 2.5.2: Scheme of the constitutive relation between ϕ and $\overline{\phi}$

Note that (2.53) can be transformed into the following relation between ρ_p and η_p.

$$\begin{aligned} \eta_p(\boldsymbol{x}, t) &= \mathcal{A}_p\left(\rho_p(\boldsymbol{x}, \cdot)\right)(t), \\ \mathcal{A}_p(\xi)(t) &= \operatorname{ess\,sup}\left\{H_p\left(\xi(s)\right) \,:\, s \le t\right\}, \\ H_p(s) &= \begin{cases} 0 & \text{if } s < \rho_{p,0}, \\ a(s-\rho_{p,0}) & \text{if } s \in [\rho_{p,0}, \rho_{p,1}], \\ \eta_{\max} & \text{if } s > \rho_{p,1}, \end{cases} \end{aligned} \tag{2.54}$$

where $\rho_{p,i} = \overline{\rho_p}\,\phi_i$ for $i = 0, 1$ are the mass densities corresponding to the activation and exhaustion, respectively, and $\eta_{\max} = \overline{\rho_p} \cdot \overline{\phi}_{\max}$. Also note that $H_p(s) = \overline{\rho_p} \cdot H_\phi(s/\overline{\rho_p})$.

Remark 2.5.1. *If the equations presented in Section 2.4.4 would be used to describe the evolution of the particle density, the mass flux of particles towards the active part* Γ *would be equal to* $\dot{\boldsymbol{m}}_p = \rho_p \boldsymbol{U} = \boldsymbol{0}$ *(*$\boldsymbol{U} = \boldsymbol{0}$ *on* $\Gamma \subset \partial\Omega \setminus (\Gamma^{\text{in}} \cup \Gamma^{\text{out}})$*). Therefore, this model is not appropriate for the detection because no particles would be absorbed.*

2.5.2 Evolution of the particle density

In this section, we derive a diffusion equation for the time evolution of the particle density ρ_p. And therefore, the particle flux towards Γ is generally different from zero. To derive the diffusion equation, two approaches will be compared. In the first one, presented in [14], a diffusion equation for particles suspended in a liquid is derived from thermodynamical considerations (without using (2.25)). The second one is Smoluchowski's approximation (see [55]). Both approaches are presented in [45].

Einstein's diffusion coefficient. Assuming that the liquid in which the particles are suspended is at rest, the formula

$$\beta = \frac{R\,\theta}{N} \cdot \frac{1}{3\,\pi\,\mu\,d_p} = \frac{k\,\theta}{3\,\pi\,\mu\,d_p} \tag{2.55}$$

for the diffusion coefficient β is derived in [14, §3]. Here, N is the number of molecules in 1 g, μ the viscosity of the liquid, k Boltzmann's constant, and θ the temperature. The second expression in (2.55) can be found in [45, Chapter 4]. Taking into account the effects of the Cunningham slip correction, (2.55) becomes

$$\beta = \frac{k\,\theta\,C_c}{3\,\pi\,\mu\,d_p}. \tag{2.56}$$

Under the assumption $\boldsymbol{U} = \boldsymbol{0}$ the particle density satisfies the diffusion equation

$$\frac{\partial \rho_p}{\partial t} = \beta \Delta \rho_p, \tag{2.57}$$

see [14, §4], [45, Chapter 4] or [28, Chapter 7.4]. Integrating (2.57) over a control volume V, applying Gauss' Theorem to the right-hand side, and comparing the resulting equation with (2.15), we obtain an expression for the mass flux of the particles

$$\dot{\boldsymbol{m}}_p = -\beta\,\nabla \rho_p, \qquad \text{if } \boldsymbol{U} = \boldsymbol{0}. \tag{2.58}$$

In the case of a fluid in motion, we add the drift term $\rho_p\,\boldsymbol{U}$ to (2.58) and proceed as in Section 2.3. Analogously to (2.15), we get

$$\int_V \frac{\partial \rho_p}{\partial t}\,\mathrm{d}\boldsymbol{x} = -\int_{\partial V} \dot{\boldsymbol{m}}_p \cdot \boldsymbol{\nu}\,\mathrm{d}s = -\int_V \mathrm{div}\,(\rho_p\,\boldsymbol{U} - \beta\,\nabla \rho_p)\,\mathrm{d}\boldsymbol{x}, \tag{2.59}$$

after applying Gauss' Theorem, which holds for an arbitrary volume V. Assuming ρ_p and $\boldsymbol{U}$ are sufficiently regular, we deduce the conservation of mass for the particles:

$$(\rho_p)_t + \mathrm{div}\,(\rho_p\,\boldsymbol{U}) - \beta\,\Delta \rho_p = 0. \tag{2.60}$$

Smoluchowski's approximation. According to [45] we consider the Smoluchowski approximation of a Brownian particle

$$\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{U}(\boldsymbol{x}(t), t)\,\mathrm{d}t + \bar{\beta}\,\mathrm{d}\boldsymbol{W}_t, \qquad \text{with } \bar{\beta} := \frac{\beta_*}{\alpha}. \tag{2.61}$$

In (2.61), $\boldsymbol{x}(t)$ denotes the position of the observed particle at time t, $\boldsymbol{U}$ the velocity of the ambient fluid, and $\boldsymbol{W}_t$ a Wiener-process. To obtain (2.61) from equations (2.28), we formally use the following

Theorem 2.5.2 ([45, Theorem 10.1])**.** *Let $\boldsymbol{b} : \mathbb{R}^l \to \mathbb{R}^l$ satisfy a global Lipschitz condition, and let $\boldsymbol{W}$ be a Wiener process on $\mathbb{R}^l$. Let $\boldsymbol{x}, \boldsymbol{V}$ be a solution of the coupled equations*

$$\begin{aligned} \mathrm{d}\boldsymbol{x}(t) &= \boldsymbol{V}(t)\,\mathrm{d}t; & \boldsymbol{x}(0) &= \boldsymbol{x}^0, \\ \mathrm{d}\boldsymbol{V}(t) &= -\alpha\,\boldsymbol{V}(t)\,\mathrm{d}t + \alpha\,\boldsymbol{b}\left(\boldsymbol{x}(t)\right)\,\mathrm{d}t + \alpha\,\mathrm{d}\boldsymbol{W}_t; & \boldsymbol{V}(0) &= \boldsymbol{V}^0. \end{aligned}$$

Let $\boldsymbol{y}$ be a solution of

$$\mathrm{d}\boldsymbol{y}(t) = \boldsymbol{b}\left(\boldsymbol{y}(t)\right)\,\mathrm{d}t + \mathrm{d}\boldsymbol{W}_t; \qquad \boldsymbol{y}(0) = \boldsymbol{x}^0.$$

Then, for all $\boldsymbol{V}^0$, with probability one

$$\lim_{\alpha\to\infty} \boldsymbol{x}(t) = \boldsymbol{y}(t),$$

uniformly for t in compact subintervals of $[0, \infty)$.

It is noted in [45] that the theorem remains valid for the case that $\boldsymbol{b}$ is continuous and, for t in compact sets, satisfies a uniform Lipschitz condition in $\boldsymbol{x}$. Actually, α given by (2.27) is large but finite (see Table 2.6.4). Therefore, we formally apply the theorem to system (2.28) where $\bar{\beta} = \beta_*/\alpha$ is a new coefficient. This yields (2.61) and we will show, that (2.60) follows from (2.61).

Denote by $p(s, \boldsymbol{y}, t, \boldsymbol{x})$ the transition probability density when a particle starting at time s from a point $\boldsymbol{y}$, moving according to (2.61), arrives at time $t > s$ at the point $\boldsymbol{x}$. Thus, $\rho_p(\boldsymbol{x}, t)$ can be computed from the particle density at time s by:

$$\rho_p(\boldsymbol{x}, t) = \int_{\mathbb{R}^N} \rho_p(\boldsymbol{y}, s)\, p(s, \boldsymbol{y}, t, \boldsymbol{x})\, \mathrm{d}\boldsymbol{y}. \tag{2.62}$$

To derive an evolution equation for ρ_p, apply Theorem 2.C.4 to (2.62) to obtain the conservation equation for the particle density:

$$(\rho_p)_t + \operatorname{div}\left(\rho_p\, \boldsymbol{U}\right) = \beta_S\, \Delta\rho_p,$$

where the diffusion coefficient is given by

$$\beta_S := \frac{\bar{\beta}^2}{2} = \frac{113}{324} \cdot \frac{k\,\theta\,C_c}{\pi\,\mu\,d_p}. \tag{2.63}$$

Expression (2.63) is obtained by using (2.27) to compute $\bar{\beta}$ from (2.61), and expressing the particle mass by $m_p = \rho_p\,\pi\,d_p^3/6$.

Remark 2.5.3. *Note that both derivations are not completely rigorous in strong sense. First, diffusion equation* (2.60) *is derived from* (2.57) *ignoring the assumption that the fluid is at rest. Second, Theorem 2.5.2 is applied to get* (2.61) *in the case of large but finite α. To justify these procedures compare the diffusion coefficients of* (2.56) *and* (2.63)

$$\beta_S \approx 1.05 \cdot \beta.$$

Since both approaches yield nearly the same result, we accept both of them but use preferably the value of β given by (2.56).

Boundary conditions. From (2.59), one can deduce an expression for the mass flux of particles

$$\dot{\boldsymbol{m}}_p = \rho_p \, \boldsymbol{U} - \beta \, \nabla \rho_p. \tag{2.64}$$

Inserting (2.64) into (2.51) yields the boundary condition for ρ_p

$$(\eta_p)_t = -\beta \, \partial_{\boldsymbol{\nu}} \rho_p, \tag{2.65}$$

because $\boldsymbol{U} = \boldsymbol{0}$ on Γ. Combing (2.60) with (2.65) and adding boundary conditions on $\partial\Omega \setminus \Gamma$ and initial values for ρ_p and η_p yields the following initial boundary value problem

$$\begin{aligned}
(\rho_p)_t + \operatorname{div}(\rho_p \, \boldsymbol{U}) - \beta \, \Delta \rho_p = 0 \qquad & \text{in } \Omega \times (0,T), \\
(\eta_p)_t = -\beta \, \partial_{\boldsymbol{\nu}} \rho_p, \quad \eta_p = \mathcal{A}(\rho_p) \qquad & \text{on } \Gamma \times (0,T), \\
-\left[\rho_p \, \boldsymbol{U} - \beta \nabla \rho_p\right] \cdot \boldsymbol{\nu} = -g_p \, \boldsymbol{U} \cdot \boldsymbol{\nu} \qquad & \text{on } \Gamma^{\text{in}} \times (0,T), \\
-\partial_{\boldsymbol{\nu}} \rho_p = 0 \qquad & \text{on } \left[\partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}})\right] \times (0,T), \\
\rho_p(\boldsymbol{x},0) = \rho_p^0(\boldsymbol{x}), \qquad \eta_p(\boldsymbol{x},0) = \eta_p^0(\boldsymbol{x}) \qquad & \text{for } t = 0.
\end{aligned} \tag{2.66}$$

On the inlet, the mass flux of particles $\dot{\boldsymbol{m}}_p \cdot (-\boldsymbol{\nu})$ into the wet cell is prescribed by $g_p \, \boldsymbol{U} \cdot (-\boldsymbol{\nu})$, where g_p is assumed to be a known function. The boundary part $\partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}} \cup \Gamma^{\text{out}})$ is assumed to be solid. Therefore, it is reasonable to assume that the velocity field of the liquid satisfies the no-slip condition ($\boldsymbol{U} = \boldsymbol{0}$) on this part. By formula (2.64), the condition $-\partial_{\boldsymbol{\nu}} \rho_p = 0$ means that the particles cannot leave the wet cell through solid walls. In contrast to the inflow condition, the boundary condition $-\partial_{\boldsymbol{\nu}} \rho_p = 0$ is also imposed on the outlet Γ^{out}. This means that the diffusion does not contribute to the outflow, and the mass flux of particles through the outlet is determined by the transport term $\rho_p \, \boldsymbol{U} \cdot \boldsymbol{\nu}$ only.

Now, assume that the liquid is weakly compressible as in Section 2.3, i.e. all products containing $\operatorname{div} \boldsymbol{U}$ (see (2.10)) are neglected. Then, the approximation $\operatorname{div}(\rho_p \, \boldsymbol{U}) \approx \boldsymbol{U} \cdot \nabla \rho_p$ holds, and we see that the system of equations (2.4) describing the decoupled measurement problem consists of system (2.66) and flow problem (2.1).

In Section 3.4.2, we show that these conditions are reasonable initial and boundary data.

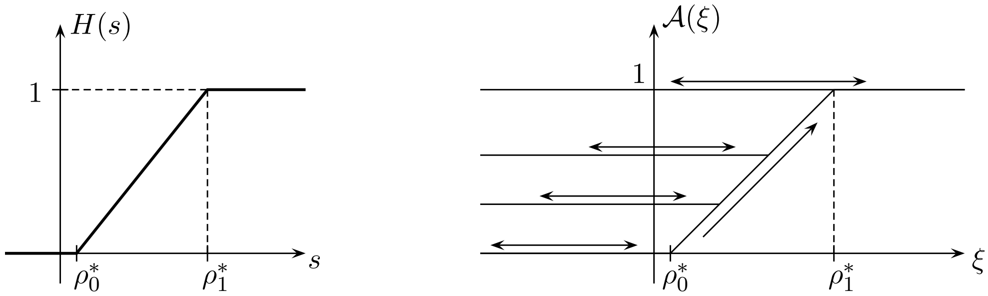
Rescaling. To simplify the notation for theoretical investigations, system (2.66) is rescaled. First, to reduce the diffusion coefficient to 1, introduce new time and velocity scales: $t' = \beta \, t$ and $\boldsymbol{U}' = \beta^{-1} \, \boldsymbol{U}$. Second, to obtain a maximal value of the surface mass density to be equal to 1, define the new variables $\eta = \eta_p / \eta_{\max}$ and $\rho = \rho_p / \eta_{\max}$, which satisfy

$$\eta_t = -\partial_{\boldsymbol{\nu}} \rho \qquad \text{on } \Gamma,$$

where (similar to the transition from (2.52) to (2.54))

$$\begin{aligned}
\eta(\boldsymbol{x},t) &= \mathcal{A}\left(\rho(\boldsymbol{x},\cdot)\right)(t), \\
\mathcal{A}(\xi)(t) &= \operatorname{ess\,sup}\left\{H\left(\xi(\tau)\right) \,:\, \tau \le t\right\}, \\
H(s) &= \begin{cases} 0 & \text{if } s < \rho_0^*, \\ a(s - \rho_0^*) & \text{if } s \in [\rho_0^*, \, \rho_1^*], \\ 1 & \text{if } s > \rho_1^*. \end{cases}
\end{aligned} \tag{2.67}$$

The constants are given by $\rho_i^* = (\overline{\rho_p}/\eta_{\max})\,\phi_i,\ i = 1, 2,\ a = (\rho_1^* - \rho_0^*)^{-1}$. The graph of the function H and the action of the operator $\mathcal{A}$ are shown in Figure 2.5.3.



2.5.3.a: Graph of H

2.5.3.b: Action of the hysteresis operator $\mathcal{A}$

Figure 2.5.3: The constitutive relations for the scaled variables

Finally, setting $g = g_p/\eta_{\max}$, dropping the primes, and assuming the liquid being weakly compressible, wee see that system (2.66) yields (2.5) describing the evolution of the particle density.

2.5.3 Influence of the particles on the liquid

The influence of the liquid onto the particles is already modeled for the measurement part in Section 2.5.2. In the same way as for the transport problem in Section 2.4.3, we are going to derive a simple description of the influence of the particles on the liquid. To this end, a conservation equation for the total momentum is derived similar to [33, X.4]. Our basic assumptions in this section are that the Korteweg stresses can be neglected, and that the volume fraction of the particles is small compared to the fraction of the liquid. A mathematical argument for the first assumption is given in the beginning of Section 1.4. To provide a physical justification, we note that Korteweg developed his idea of the stress induced by composition gradients for mixtures that are in equilibrium with external body forces. However, in flowing mixtures, the dynamics induced by the motion of the mixture occur in shorter time scales than the dynamics induced by the diffusive effects (unless the velocity is extremely small). Therefore, it is reasonable to assume that the stress induced by composition gradients does not significantly affect the dynamics in situations we are going to consider.

Let us implement the above sketched objectives. According to [33] and similar to Section 2.5.1 denote by ϕ the volume fraction of particles. We assume that the density ρ_f of the composite is given by the so called simple mixture equation

$$\rho_f(\phi) = \overline{\rho_l}\,(1-\phi) + \overline{\rho_p}\;\phi, \tag{2.68}$$

where $\overline{\rho_l}$ and $\overline{\rho_p}$ denote the proper densities of the liquid and particles, respectively as before. Further, let $\boldsymbol{V}_l$ and $\boldsymbol{V}_p$ denote the average velocities of the liquid and particles. Set

$$\boldsymbol{V}_m = \frac{\overline{\rho_l}\,\boldsymbol{V}_l\,(1-\phi) + \overline{\rho_p}\,\boldsymbol{V}_p\,\phi}{\overline{\rho_l}\,(1-\phi) + \overline{\rho_p}\;\phi}. \tag{2.69}$$

By [33, X.4], ρ_f and $\boldsymbol{V}_m$ satisfy the continuity equation and the conservation of momentum:

$$\begin{aligned} \frac{\mathrm{d}\rho_f}{\mathrm{d}t} &= -\rho_f \operatorname{div} \boldsymbol{V}_m, \\ \rho_f \frac{\mathrm{d}\boldsymbol{V}_m}{\mathrm{d}t} &= -\nabla p + \operatorname{div} \Pi^D + \rho_f \boldsymbol{F}, \end{aligned} \tag{2.70}$$

where p is the pressure of the mixture. In (2.70), the tensor Π^D is the sum of a “Newtonian part” and a part which is given in terms of the Korteweg stresses:

$$\Pi^D = \mu \left[\left(\nabla \boldsymbol{V}_m + [\nabla \boldsymbol{V}_m]^T \right) - \frac{2}{3} \operatorname{div} (\boldsymbol{V}_m) \cdot \mathbb{I} \right] + \mathbb{T},$$

with

$$\mathbb{T} = \mathbb{T}^K - \frac{1}{3} \operatorname{trace}(\mathbb{T}^K) \cdot \mathbb{I},$$

and $\mathbb{T}^K$ denotes the Korteweg stress tensor (see formula (1.1)). By our assumptions, $\mathbb{T}$ can be neglected.

Next, we identify the averaged variables with the ones used in Sections 2.5.1 and 2.5.2. In simple mixtures, the densities ρ_l and ρ_p of the liquid and the particle phase are given in terms of the proper densities $\overline{\rho_l}$, $\overline{\rho_p}$, and the volume fraction ϕ by

$$\rho_l = \overline{\rho_l}\,(1-\phi), \qquad \rho_p = \overline{\rho_p}\,\phi. \tag{2.71}$$

Further, $\boldsymbol{V}_l$ can be identified with $\boldsymbol{U}$. Evaluating the substantial derivative on the left-hand side of the momentum equation in (2.70) and using (2.15) for the mass flux of the liquid and (2.64) for the mass flux of the particle phase yield the relations

$$\rho_f \boldsymbol{V}_m = \dot{\boldsymbol{m}}_f = \dot{\boldsymbol{m}}_l + \dot{\boldsymbol{m}}_p = \rho_l \boldsymbol{U} + \rho_p \boldsymbol{U} - \beta \nabla \rho_p. \tag{2.72}$$

Rewrite the left-hand side of the momentum equation of (2.70) similar to (2.23) where the case of a single fluid phase was considered and use (2.72) to obtain

$$\rho_f \frac{\mathrm{d}\boldsymbol{V}_m}{\mathrm{d}t} = \rho_f (\boldsymbol{V}_m)_t + \left([\rho_l \boldsymbol{U} + \rho_p \boldsymbol{U} - \beta \nabla \rho_p] \cdot \nabla \right) \boldsymbol{V}_m. \tag{2.73}$$

By our assumptions, ϕ is small so that (2.69) yields the approximation

$$\boldsymbol{V}_m \approx \boldsymbol{V}_l = \boldsymbol{U}. \tag{2.74}$$

To identify the pressure, we argue similar to Section 2.4.3: since ϕ is supposed to be small, the particles can not significantly contribute to the formation of the pressure. Thus, p can be identified with the pressure of the liquid. Additionally, the approximation (2.74) yields $-\nabla p + \operatorname{div} \Pi^D = \operatorname{div} \Pi$ (see (2.22)). Rewriting the continuity equation of (2.70) as $(\rho_f)_t + \operatorname{div} \dot{\boldsymbol{m}}_f = 0$ and inserting (2.68), (2.71), (2.72), and (2.60) yield a continuity equation for ρ_l and $\boldsymbol{U}$. Thus, inserting (2.73) and (2.74) into the momentum equation of (2.70) and accounting for (2.60) yield the following system of equations:

$$\begin{aligned} (\rho_l)_t + \operatorname{div} (\rho_l \boldsymbol{U}) &= 0, \\ (\rho_p)_t + \operatorname{div} (\rho_p \boldsymbol{U} - \beta \nabla \rho_p) &= 0, \\ (\rho_l + \rho_p) \boldsymbol{U}_t + \big([\rho_l \boldsymbol{U} + \rho_p \boldsymbol{U} - \beta \nabla \rho_p] \cdot \nabla \big) \boldsymbol{U} &= \operatorname{div} \Pi + (\rho_l + \rho_p) \boldsymbol{F}. \end{aligned} \tag{2.75}$$

To complete the derivation of equations (2.3) for the coupled measurement problem, multiply the first and second equations in (2.75) by $\boldsymbol{U}$ and add them to the third one to obtain:

$$\big([\rho_l + \rho_p]\,\boldsymbol{U}\big)_t + \operatorname{div}\left(\boldsymbol{U} \otimes [\rho_l\,\boldsymbol{U} + \rho_p\,\boldsymbol{U} - \beta\,\nabla\rho_p]\right) = \operatorname{div}\Pi + (\rho_l + \rho_p)\,\boldsymbol{F}. \tag{2.76}$$

Now, neglect ρ_p in the first term of the left-hand side and in the last term of the right-hand side and remember the weak compressibility of the liquid to obtain (2.3).

Let us now derive a momentum equation that is different from (2.76) and the third one of (2.75). Assume summation over repeated indices and use the continuity equation of (2.70) to rewrite the j-th component of the momentum equation as follows:

$$(\rho_f\,V_{m,j})_t + \operatorname{div}\left(\rho_f\,V_{m,j}\,\boldsymbol{V}_m\right) = \frac{\partial \Pi_{jk}}{\partial x_k} + F_j, \qquad j = 1, ..., N. \tag{2.77}$$

Substitute

$$\rho_f\,V_{m,j} = \dot{m}_{f,j} = \rho_f\,U_j + \beta\,\frac{\partial \rho_p}{\partial x_j}$$

(see (2.72)) into the divergence term of (2.77) and then identify $\boldsymbol{V}_m = \boldsymbol{U}$ (see (2.74)). This yields

$$(\rho_f\,\boldsymbol{U})_t + \operatorname{div}\left([\rho_f\,\boldsymbol{U} - \beta\,\nabla\rho_p] \otimes \boldsymbol{U}\right) = \operatorname{div}\Pi + \rho_f\,\boldsymbol{F}. \tag{2.78}$$

Equations (2.76) and (2.78) differ in the convective terms only due to (2.68) and (2.71).

Remark 2.5.4. *The momentum equations* (2.76) *and* (2.78) *are derived under the same assumptions and approximations. Nevertheless, we prefer to use* (2.76) *instead of* (2.78) *for the derivation of equations for the coupled measurement problem because of the following reasons. First, the derivation of* (2.76) *from system* (2.75) *is consistent with the form of system* (2.70)*. Second, equation* (2.76) *yields a conventional equality for the kinetic energy like in the case of single fluid flow. Such relations are useful in the analysis of flow problems for incompressible or compressible media. See for example [17, 18, 36, 38, 40, 41, 47, 60].*

Show first the consistency claimed in the remark. Evaluating the total derivative on the left-hand side of the second equation of (2.70), adding the continuity equation multiplied by $\boldsymbol{V}_m$, and applying the identification (2.72) yield the identity

$$\rho_f\,(\boldsymbol{V}_m)_t + (\dot{\boldsymbol{m}}_f \cdot \nabla)\boldsymbol{V}_m = (\rho_f\,\boldsymbol{V}_m)_t + \operatorname{div}\left(\boldsymbol{V}_m \otimes \dot{\boldsymbol{m}}_f\right). \tag{2.79}$$

The same method is used to derive (2.76) from the system (2.75). The left-hand side of the momentum equation of (2.75) is analogous to the left-hand side of (2.79) and the left-hand side of (2.76) is analogous to the right-hand side of (2.79). This method does not work if (2.76) is replaced by (2.78) since the gradient $\nabla\rho_p$ appears in the convective terms.

Next, show the claim on the equality for the kinetic energy in Remark 2.5.4. It follows from a general formula. Let the functions

$$a,\, f : \Omega \times [0,T] \to \mathbb{R} \qquad \text{and} \qquad \boldsymbol{b},\, \boldsymbol{u} : \Omega \times [0,T] \to \mathbb{R}^N$$

be (componentwisely) in $\mathcal{C}^1\big(\Omega \times (0,T)\big)$. Moreover, let a, f and $\boldsymbol{b}$ satisfy

$$a_t + \operatorname{div}\boldsymbol{b} = f. \tag{2.80}$$

Then, the following computation holds:

$$\begin{aligned}
[(a\,\boldsymbol{u})_t + \operatorname{div}(\boldsymbol{u}\otimes\boldsymbol{b})]\cdot\boldsymbol{u} &= |\boldsymbol{u}|^2\,a_t + |\boldsymbol{u}|^2\,\frac{\partial b_k}{\partial x_k} + \frac{a}{2}\,\frac{\partial|\boldsymbol{u}|^2}{\partial t} + \frac{b_k}{2}\,\frac{\partial|\boldsymbol{u}|^2}{\partial x_k}\\
&= |\boldsymbol{u}|^2\,f + \frac{a}{2}\frac{\partial|\boldsymbol{u}|^2}{\partial t} + \frac{1}{2}\,\frac{\partial(|\boldsymbol{u}|^2\,b_k)}{\partial x_k} - \frac{|\boldsymbol{u}|^2}{2}\,\frac{\partial b_k}{\partial x_k}\\
&= \frac{1}{2}\left[\left(a\,|\boldsymbol{u}|^2\right)_t + \operatorname{div}\left(|\boldsymbol{u}|^2\boldsymbol{b}\right) + |\boldsymbol{u}|^2\,f\right].
\end{aligned} \tag{2.81}$$

Adding both mass conservations in (2.75) and using (2.72) yields

$$(\rho_f)_t + \operatorname{div}(\dot{\boldsymbol{m}}_f) = 0,$$

which is similar to (2.80). Suppose $\boldsymbol{U} = \boldsymbol{0}$ on $\partial\Omega$ and multiply (2.76) by $\boldsymbol{U}$. Use (2.80), (2.81) with $(a,\,f,\,\boldsymbol{b},\,\boldsymbol{u}) = (\rho_f,\,0,\,\dot{\boldsymbol{m}}_f,\,\boldsymbol{U})$ on the left-hand side and integrate over Ω to obtain the energy equation

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho_f\,|\boldsymbol{U}|^2\,\mathrm{d}\boldsymbol{x} + \int_\Omega\left[\mu|\nabla\boldsymbol{U}|^2 + \xi|\operatorname{div}\boldsymbol{U}|^2\right]\mathrm{d}\boldsymbol{x} = \int_\Omega\left[\rho_f\boldsymbol{F} - \nabla p\right]\cdot\boldsymbol{U}\,\mathrm{d}\boldsymbol{x}.$$

This equation is analogous to [41, Equation (5.9)], for example.

Thus, the argumentation in Remark 2.5.4 is grounded.

2.6 Physical constants

In this section, we give the values of physical constants which we used in the previous sections. Values given in Tables 2.6.1, 2.6.2 and 2.6.3 can be found in [28, Appendix A1] and [58, Appendix D].

Table 2.6.1: Physical constants

Boltzmann's constant k	$1.38\,\mathrm{E}-23\ \mathrm{N}\cdot\mathrm{m}\cdot\mathrm{K}^{-1}$
Gas constant R	$8.314\ \mathrm{J}\cdot\mathrm{mol}^{-1}\cdot\mathrm{K}^{-1}$
Molar Volume V_{mol} of ideal gas at 20 $°C$	$2.24\,\mathrm{E}-2\,\mathrm{m}^3\cdot\mathrm{mol}^{-1}$
Density of titanium dioxide TiO_2	$4.23\,\mathrm{E}+3\ \mathrm{kg}\cdot\mathrm{m}^{-3}$

Table 2.6.2: Properties of water at 20 $°C$ and $1\ \mathrm{atm} = 1.01\,\mathrm{E}+5\ \mathrm{Pa}$

Dynamic viscosity μ	$1000.\ \mathrm{E}-6\ \mathrm{kg}\cdot\mathrm{m}^{-1}\cdot\mathrm{s}^{-1}$
Kinematic viscosity ν	$1.000\ \mathrm{E}-6\ \mathrm{m}^2\cdot\mathrm{s}^{-1}$
Density ρ_0	$1.000\ \mathrm{E}+3\ \mathrm{kg}\cdot\mathrm{m}^{-3}$

An ideal gas is characterized by the relation

$$p = \frac{n_{\mathrm{mol}}}{V}\cdot R\cdot\theta = \rho\cdot\frac{R}{m_{\mathrm{mol}}}\cdot\theta,$$

Table 2.6.3: Properties of dry air at 20 °C and $1 \text{ atm} = 1.01 \text{ E} + 5 \text{ Pa}$

Density ρ_0	$1.205 \text{ kg} \cdot \text{m}^{-3}$
Dynamic viscosity μ	$1.81 \text{ E} - 5 \text{ Pa} \cdot \text{s}$
Mean free path λ	$0.066\ \mu\text{m}$
Compressibility γ_{ideal}	$1. \text{ E} - 5 \text{ m} \cdot \text{s}^2 \cdot \text{kg}^{-1}$

where V, n_{mol} and m_{mol} denote the volume occupied by the gas, the number of moles contained in V, and the molar mass of the gas, respectively. For such gases, the compressibility γ_{ideal} (see Section 2.3) is given by

$$\gamma_{\text{ideal}} = \frac{V_{\text{mol}}}{R \cdot \theta}$$

where V_{mol} is the molar volume of the gas.

Values of the Cunningham slip correction C_c and the diffusion coefficient β in air given in Table 2.6.4 can be found in [28, Appendix A11]. The values of α and β_* are computed using (2.27), and the values of β in water are computed using (2.55).

Table 2.6.4: Physical properties of spherical titanium dioxide particles depending on the diameter

Particle diameter and mass	Property	in Air	in Water
$d_p = 1\ \mu\text{m}$, $m_p = 2.12 \text{ E} - 15 \text{ kg}$	C_c	1.165	—
	α	$6.61 \text{ E} + 4 \text{ s}^{-1}$	$4.26 \text{ E} + 12 \text{ s}^{-1}$
	β_*	$0.49 \text{ m} \cdot \text{s}^{-3/2}$	$3.94 \text{ E} + 3 \text{ m} \cdot \text{s}^{-3/2}$
	β	$2.76 \text{ E} - 11 \text{ m}^2 \cdot \text{s}^{-1}$	$4.29 \text{ E} - 19 \text{ m}^2 \cdot \text{s}^{-1}$
$d_p = 0.1\ \mu\text{m}$, $m_p = 2.21 \text{ E} - 18 \text{ kg}$	C_c	2.888	—
	α	$2.67 \text{ E} + 6\text{s}^{-1}$	$4.26 \text{ E} + 14 \text{ s}^{-1}$
	β_*	$9.87 \text{ E} + 1 \text{ s}^{-3/2}$	$1.25 \text{ E} + 6 \text{ m} \cdot \text{s}^{-3/2}$
	β	$6.85 \text{ E} - 10 \text{ m}^2 \cdot \text{s}^{-1}$	$4.29 \text{ E} - 18 \text{ m}^2 \cdot \text{s}^{-1}$
$d_p = 0.01\ \mu\text{m}$, $m_p = 2.21 \text{ E} - 21 \text{ kg}$	C_c	22.447	—
	α	$3.43 \text{ E} + 7 \text{ s}^{-1}$	$4.26 \text{ E} + 16 \text{ s}^{-1}$
	β_*	$1.12 \text{ E} + 4 \text{ m} \cdot \text{s}^{-3/2}$	$3.94 \text{ E} + 8 \text{ m} \cdot \text{s}^{-3/2}$
	β	$5.31 \text{ E} - 8 \text{ m}^2 \cdot \text{s}^{-1}$	$4.29 \text{ E} - 17 \text{ m}^2 \cdot \text{s}^{-1}$

In [28, Chapter 3.4], the Cunningham correction factor C_c (see Sections 2.4.1 and 2.5.2) is specified as

$$C_c = \begin{cases} 1 & d_p > 1\ \mu\text{m}, \\ 1 + 2.52\,(\lambda/d_p) & 0.1\ \mu\text{m} < d_p < 1\ \mu\text{m}, \\ 1 + (\lambda/d_p)\,[2.514 + 0.800\ \exp\left(-0.55\, d_p/\lambda\right)] & d_p < 0.01\ \mu\text{m}, \end{cases} \tag{2.82}$$

where λ is the mean free path. See also [21, Chapter 2].

2.A The Transport Theorem

Let $(0, T)$ be a time interval, during which we follow the fluid motion, and $\Omega_t \subset \mathbb{R}^N$ denote the domain occupied by the fluid at time $t \in (0, T)$. Then the domain of definition of the quantities describing the flow is the set

$$\mathcal{M} = \{(\boldsymbol{x}, t)\ :\ \boldsymbol{x} \in \Omega_t\,,\ t \in (0, T)\} \subset \mathbb{R}^{N+1}.$$

In the Lagrangian description the trajectories of the fluid particles are determined by the equation

$$\boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X}, t), \tag{2.83}$$

where $\boldsymbol{X}$ represents the reference determining the particle under consideration. Usually one assumes that $\boldsymbol{X}$ is the initial position of the particle, i.e. $\boldsymbol{X} = \boldsymbol{\phi}(\boldsymbol{X}, 0)$. The velocity and acceleration of the particle referenced by $\boldsymbol{X}$ are given by

$$\widehat{\boldsymbol{U}}(\boldsymbol{X}, t) = \frac{\partial \boldsymbol{\phi}(\boldsymbol{X}, t)}{\partial t} \qquad \text{and} \qquad \widehat{\boldsymbol{a}}(\boldsymbol{X}, t) = \frac{\partial^2 \boldsymbol{\phi}(\boldsymbol{X}, t)}{\partial t^2}, \tag{2.84}$$

provided the above derivatives exist.

The Eulerian description is based on the determination of the velocity $\boldsymbol{U}(\boldsymbol{x}, t)$ of the fluid particle passing through the point $\boldsymbol{x} \in \Omega_t$ at time t. Due to (2.83) and (2.84), we get the relation

$$\boldsymbol{U}(\boldsymbol{x}, t) = \widehat{\boldsymbol{U}}(\boldsymbol{X}, t) \qquad \text{where} \qquad \boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X}, t).$$

If (2.87) is satisfied, the acceleration of the fluid particle passing through $\boldsymbol{x}$ at time t is expressed as

$$\boldsymbol{a} = \boldsymbol{U}_t + (\boldsymbol{U} \cdot \nabla)\,\boldsymbol{U} \qquad \text{or} \qquad a_j(\boldsymbol{x}, t) = \frac{\partial U_j}{\partial t} + U_k \cdot \frac{\partial U_j}{\partial x_k},$$

where $\boldsymbol{a} = (a_1, a_2, a_3)$, $\boldsymbol{U} = (U_1, U_2, U_3)$, $\boldsymbol{x} = (x_1, x_2, x_3)$, and the summation convention was used. Note that the trajectory of the particle passing through the point $\boldsymbol{X} \in \Omega_{t_0}$ at time $t_0 \in (0, T)$ is given in Eulerian coordinates by the initial value problem

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{U}(\boldsymbol{x}, t)\ , \qquad \boldsymbol{x}(t_0) = \boldsymbol{X}.$$

To account for the dependence on t_0, rewrite (2.83) in the form

$$\boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X}, t_0; t), \tag{2.85}$$

then, the problem (2.85) can be rewritten as

$$\frac{\partial \boldsymbol{x}(\boldsymbol{X}, t_0;\, t)}{\partial t} = \boldsymbol{U}(\boldsymbol{x}(\boldsymbol{X}, t_0;\, t),\, t), \qquad \boldsymbol{x}(\boldsymbol{X}, t_0;\, t_0) = \boldsymbol{X}. \tag{2.86}$$

In the following we will assume that the velocity is continuously differentiable

$$\boldsymbol{U} \in \mathcal{C}^1 (\mathcal{M})^3 . \tag{2.87}$$

Theorem 2.A.1 ([18, 1.3.22 Theorem])**.** *Assume* (2.87)*, then the following statements hold:*

1. *For each* $(\boldsymbol{X}, t_0) \in \mathcal{M}$ *problem* (2.86) *has exactly one maximal solution* $\boldsymbol{\phi}(\boldsymbol{X}, t_0; t)$ *(defined for t from a certain interval* $(\alpha_{\boldsymbol{X},t_0}, \beta_{\boldsymbol{X},t_0})$*).*

2. *The mapping* $\boldsymbol{\phi}$ *has continuous first order partial derivatives with respect to* $X_i, t_0, t,\ i = 1, ..., N$ *and continuous derivatives* $\partial^2 \boldsymbol{\phi}/\partial t\, \partial X_i,\ \partial^2 \boldsymbol{\phi}/\partial t_0\, \partial X_i,\ i = 1, ..., N$ *in its domain of definition* $\{(\boldsymbol{X}, t_0; t) : (\boldsymbol{X}, t_0) \in \mathcal{M},\ t \in (\alpha_{\boldsymbol{X},t_0}, \beta_{\boldsymbol{X},t_0})\}$.

For $V(t_0) \subset \Omega_{t_0}$ denote by $V(t) := \{\boldsymbol{x} : \boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X}, t_0;\, t)$ for some $\boldsymbol{X} \in V(t_0)\}$ the set occupied by the same particles at time t.

Lemma 2.A.2 ([18, 1.4.5 Lemma])**.** *Let* $t_0 \in (0, T)$*,* $V(t_0)$ *be a bounded domain with* $\overline{V(t_0)} \subset \Omega_{t_0}$*. Then there exists an interval* $(t_1, t_2) \ni t_0$ *such that the following conditions are satisfied:*

1. *The mapping "*$t \in (t_1, t_2), \boldsymbol{X} \in V(t_0) \mapsto \boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X}, t_0;\, t) \in V(t)$*" has continuous first order derivatives with respect to* t, X_i *and continuous second order derivatives* $\partial^2 \boldsymbol{\phi}/\partial t \partial X_i, i = 1, ..., N$.

2. *The mapping "*$\boldsymbol{X} \in V(t_0) \mapsto \boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X}, t_0;\, t) \in V(t)$*" is a continuously differentiable one-to-one mapping of* $V(t_0)$ *onto* $V(t)$ *with continuous and bounded Jacobian determinant*
$$J(\boldsymbol{X}, t) = \det \left(\frac{\partial \boldsymbol{\phi}(\boldsymbol{X}, t_0;\, t)}{\partial \boldsymbol{X}} \right) > 0 \qquad \forall \boldsymbol{X} \in V(t_0),\, \forall t \in (t_1, t_2).$$

3. *The inclusion*
$$\left\{ (\boldsymbol{x}, t) :\ t \in [t_1, t_2],\, \boldsymbol{x} \in \overline{V(t)} \right\} \subset \mathcal{M}$$
holds and thus, the mapping $\boldsymbol{U}$ *has continuous and bounded first order derivatives on* $\{(\boldsymbol{x}, t) :\ t \in (t_1, t_2),\, \boldsymbol{x} \in V(t)\}$.

4. $$\boldsymbol{U}(\boldsymbol{\phi}(\boldsymbol{X}, t_0;\, t), t) = \frac{\partial \boldsymbol{\phi}(\boldsymbol{X}, t_0;\, t)}{\partial t} \quad \forall \boldsymbol{X} \in V(t_0),\, \forall t \in (t_1, t_2).$$

Theorem 2.A.3 (Transport Theorem)**.** *Let the conditions 1 – 4 of Lemma 2.A.2 be satisfied and let the function* $F = F(\boldsymbol{x}, t)$ *have continuous and bounded first order derivatives on the set* $\{(\boldsymbol{x}, t) :\ t \in (t_1, t_2),\, \boldsymbol{x} \in V(t)\}$*. Then for each* $t \in (t_1, t_2)$ *there exists a finite derivative*

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V(t)} F(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} = \int_{V(t)} \left[\frac{\partial F}{\partial t}(\boldsymbol{x}, t) + \boldsymbol{U}(\boldsymbol{x}, t) \cdot \nabla F(\boldsymbol{x}, t) + F(\boldsymbol{x}, t)\, \operatorname{div} \boldsymbol{U}(\boldsymbol{x}, t) \right] \mathrm{d}\boldsymbol{x}$$
$$= \int_{V(t)} \frac{\partial F}{\partial t}(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} + \int_{\partial V(t)} F(\boldsymbol{x}, t)\, \boldsymbol{U}(\boldsymbol{x}, t) \cdot \boldsymbol{\nu}(\boldsymbol{x})\, \mathrm{d}s$$

Proof. See [18, 1.4.9 Theorem and formulas 1.4.12, 1.4.13] □

2.B The stress tensor

Assume that ρ_f, $U_i, \Pi_{ij} \in \mathcal{C}^1(\mathcal{M})$ and $f_i \in \mathcal{C}(\mathcal{M})$. The law of conservation of the moment of momentum can be formulated in the following way: *The rate of change of the moment of momentum of the piece of fluid occupying the volume $V(t)$ at any time t is equal to the sum of moments of the volume and surface forces acting on this volume.*

Using this law, one can proof the following

Theorem 2.B.1 (Symmetry of the stress tensor)**.** *The law of conservation of the moment of momentum*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V(t)} \boldsymbol{x} \times (\rho_f\, \boldsymbol{U})(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x} = \int_{V(t)} \boldsymbol{x} \times (\rho_f\, \boldsymbol{f})(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x} + \int_{\partial V(t)} \boldsymbol{x} \times \Pi \cdot \boldsymbol{\nu}\,\mathrm{d}s$$

is valid if and only if the stress tensor Π is symmetric.

Proof. [18, 1.7.30. Theorem] □

In case of Newtonian fluids, the form of the stress tensor is determined by Stokes' Postulates. To formulate them introduce the deformation velocity tensor $\mathbb{D}$ by

$$\mathbb{D} = (d_{ij})_{i,j=1}^{3}, \qquad \text{with} \qquad d_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right).$$

This is equivalent to $\mathbb{D} = (1/2)\left(\nabla \boldsymbol{U} + \nabla \boldsymbol{U}^T\right)$. Then the Stokes' Postulates read:

1. $\Pi = -p\mathbb{I} + \tau$.
2. The tensor τ is a continuous function of the deformation velocity tensor, is independent of other kinematic variables and does not explicitly depend on the position in the fluid and on time either.
3. The fluid is isotropic medium. This means that its properties are the same in all space directions.
4. If the deformation velocity tensor is zero, only the pressure force acts in the fluid. Hence, if $\mathbb{D} = 0$, then $\Pi = -p\mathbb{I}$.
5. The relation between τ and $\mathbb{D}$ is linear.

If these postulates hold then the form of Π is determined by Theorem 2.B.3.

Remark 2.B.2 (Mathematical formulation of Stokes' Postulates)**.** *The above postulates can be formulated as follows*

1. $\Pi = -p\,\mathbb{I} + \tau$.
2. $\tau = f(\mathbb{D})$, *f is continuous.*
3. *The form of the mapping f is invariant with respect to the transformation of the Cartesian coordinate system: $S\,\tau\,S^{-1} = f(S\,\mathbb{D}\,S^{-1})$ for any orthonormal matrix S.*

4. $f(0) = 0$.

5. *The mapping f is linear.*

Theorem 2.B.3 ([18, 1.7.32. Theorem]). *Under the conditions 1) - 5) of Remark 2.B.2 the stress tensor has the form*

$$\Pi = (-p + \lambda \operatorname{div} \boldsymbol{U}) \mathbb{I} + 2\mu \mathbb{D}$$

where λ, μ are constants or functions of thermodynamical quantities.

2.C Brownian motion

The following definitions can be found in [35][Section 1.5]

Definition 2.C.1 (Gaussian distribution). *Let X be a random variable*

1. *The probability measure $P_X = P \circ X^{-1}$ is called distribution of X.*

2. *For a real random variable X, the map $F_X : x \mapsto P[X \leq x]$ is called the distribution function of X (or, more accurately, of P_X). We write $X \sim \mu$ if $\mu = P_X$ and say that X has distribution μ.*

3. *A family $(X_i)_{i \in I}$ of random variables is called identically distributed if $P_{X_i} = P_{X_j}$ for all $i, j \in I$. We write $X \overset{D}{=} Y$ if $P_X = P_Y$.*

4. *Let $\mu \in \mathbb{R}, \sigma^2 > 0$ be a real random variable with*

$$F_X(x) = P[X \leq x] = \frac{1}{\sqrt{2\pi\, \sigma^2}} \int_{-\infty}^{x} \exp\left(\frac{(t-\mu)^2}{2\sigma^2} \right) \mathrm{d}t \qquad \text{for } x \in \mathbb{R}.$$

   Then

$$\mathcal{N}_{\mu,\sigma^2} := P_X$$

   is called the Gaussian normal distribution with parameters μ and σ^2. In particular $\mathcal{N}_{0,1}$, is called the standard normal distribution.

Definition 2.C.2 (Stochastic process).

1. *Let $I \subset \mathbb{R}$. A family of random variables $X = (X_t, t \in I)$ (on $(\Omega, \mathcal{F}, P)$) with values in $(E, \mathcal{E})$ is called a stochastic process with index set (or time set) I and range E.*

2. *We write $\mathcal{L}[X] = P_X$ for the distribution of X. If $\mathcal{G} \subset \mathcal{F}$ is a σ-algebra, then we write $\mathcal{L}[X|\mathcal{G}]$ for the regular conditional distribution of X given $\mathcal{G}$.*

3. *X is called a process with independent increments if X is real valued and, for all $n \in \mathbb{N}$ and all $t_0, ..., t_n \in I$ with $t_0 < \cdots < t_n$, we have*

$$\left(X_{t_i} - X_{t_{i-1}} \right)_{i=1,...,n} \text{ is independent.}$$

4. *X is called process with stationary increments if X is real-valued and*

$$\mathcal{L}[X_{s+t+r} - X_{t+r}] = \mathcal{L}[X_{s+r} - X_r] \quad \text{for all } r, s, t \in I.$$

Definition 2.C.3 (Brownian motion)**.** *A real-valued stochastic process* $B = (B_t,\, t \in [0, \infty))$ *is called a Brownian motion if*

1. $B_0 = 0$.
2. B *has independent, stationary increments.*
3. $B_t \sim \mathcal{N}_{0,t}$ *for all* $t > 0$, *and*
4. $t \mapsto B_t$ *is* P*-almost surely continuous.*

Following [45] a (vector valued) Brownian motion is also called "Wiener process" and will be denoted by $\boldsymbol{W}_t$. The next result on the transition probability density can be found in [20]. There, $\boldsymbol{\xi}$ denotes the solution of

$$\mathrm{d}\boldsymbol{\xi} = \boldsymbol{b}(\boldsymbol{\xi}(t), t)\,\mathrm{d}t + \sigma(\boldsymbol{\xi}(t), t)\,\mathrm{d}\boldsymbol{W}_t$$

The functions $\boldsymbol{b}$ and σ are supposed to satisfy

$$|\boldsymbol{b}(\boldsymbol{x}, t)| \leq C(1 + |\boldsymbol{x}|)\ , \quad |\sigma(\boldsymbol{x}, t)| \leq C(1 + |\boldsymbol{x}|) \tag{2.88}$$

on $[T_0, T] \times \mathbb{R}^N$ with a constant C. It is assumed that, for any bounded $B \subset \mathbb{R}^N$ and $T_0 < T' < T$, there exists a constant K (perhaps depending on B and T') such that, for all $\boldsymbol{x}, \boldsymbol{y} \in B$ and $T_0 \leq t \leq T'$,

$$|\boldsymbol{b}(\boldsymbol{x}, t) - \boldsymbol{b}(\boldsymbol{y}, t)| \leq K|\boldsymbol{x} - \boldsymbol{y}|\ , \quad |\sigma(\boldsymbol{x}, t) - \sigma(\boldsymbol{y}, t)| \leq K|\boldsymbol{x} - \boldsymbol{y}|, \tag{2.89}$$

holds.

Denote by p the transition probability density, that is

$$P\left(\boldsymbol{\xi}(t) \in B \,|\, \boldsymbol{\xi}(s) = y\right) = \int_B p(s, \boldsymbol{y}, t, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \qquad \text{for all } B \in \mathcal{B}(\mathbb{R}^N),$$

where $\mathcal{B}(\mathbb{R}^N)$ denotes the σ-algebra of Borel subsets of $\mathbb{R}^N$. Introduce the coefficients a_{ij} by

$$a_{ij} := \sum_{l=1}^{N} \sigma_{il}\,\sigma_{jl},$$

and for a $\Phi \in \mathcal{C}^2$ consider differential operators

$$A(t)\Phi = \frac{1}{2}\sum_{i,j=1}^{N} a_{ij}(\boldsymbol{x}, t)\frac{\partial^2\Phi}{\partial x_i \partial x_j} + \sum_{i=1}^{N} b_i(\boldsymbol{x}, t)\frac{\partial \Phi}{\partial x_i},$$

$$A^*(t)\Phi = \frac{1}{2}\sum_{i,j=1}^{N} \frac{\partial^2}{\partial x_i \partial x_j}(a_{ij}(\boldsymbol{x}, t)\Phi) - \sum_{i=1}^{N} \frac{\partial}{\partial x_i}(b_i(\boldsymbol{x}, t)\Phi).$$

The operators $\partial_t + A(t)$ and $-\partial_t + A^*(t)$ are called the "backward operator" and "forward operator", respectively.

Theorem 2.C.4 ([20, Theorem 8.1])**.** *Assume that* $\boldsymbol{b}, \sigma$ *satisfy* (2.88), (2.89) *and for* $i, j = 1, ..., N$, $b_i(\cdot, t) \in \mathcal{C}^1$ *and* $\sigma_{ij}(\cdot, t) \in \mathcal{C}^2$ *for* $T_0 \leq t \leq T$. *If* $p(s, \boldsymbol{y}, \cdot, \cdot)$ *is in* $\mathcal{C}^{1,2}((s, T) \times \mathbb{R}^N)$, *then*

$$-\frac{\partial p}{\partial t} + A^*(t)p = 0.$$

2.D The Boltzmann equation

This section provides a brief overview over the Boltzmann equation for rigid spheres. The contents is mainly taken from [11]. There, the equations of motion are given in terms of the velocities of the particles. Another possibility is to use the momentum of the particles. This approach is considered in [57].

Discussions on, for example, boundary conditions, other types of collisions, choice of the time line, regularity or ergodic hypothesis are omitted here. The interested reader is referred to [10, 11, 57, 12, 62].

To avoid difficulties at the boundary assume that a system of $K \in \mathbb{N}$ particles without internal structure is moving in infinite space $\mathbb{R}^N_x$. Under additional assumptions, which are stated below, the Boltzmann equation describes the evolution of this system on a microscopic level in terms of the one-particle distribution $f : \mathbb{R}^N_x \times \mathbb{R}^N_\xi \times I_t \to \mathbb{R}^+$.

Here $\mathbb{R}^N_x$ is the space of all possible positions of particles, $\mathbb{R}^N_\xi$ the space of all possible velocities, and I_t the (finite or infinite) time interval, where the system is considered. For any fixed time t, the quantity $f(\boldsymbol{x}, \boldsymbol{\xi}, t)\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{\xi}$ stands for the density of particles in the volume element $\mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{\xi}$ centered at the point $(\boldsymbol{x}, \boldsymbol{\xi})$ of the reduced phase space associated with the position and velocity.

The Boltzmann equation can be derived under the following assumptions (see [62, Section 1.2])

1. Particles interact via binary collisions: the gas is dilute enough so that the effect of interactions involving more than two particles can be neglected. If the gas consists of K particles of radius r in N dimensional space, this would mean

$$r^N K \ll 1\,, \qquad r^{N-1} K \simeq 1.$$

2. The collision are localized both in time and space, i.e., they are brief events which occur at a given position $\boldsymbol{x}$ and given time t.

3. The collisions are elastic: momentum and kinetic energy are preserved in a collision process.

4. The collisions are microreversible. In a deterministic setting, this means that microscopic dynamics are time-reversible. In a probabilistic setting, this means that the probability that the velocities $(\boldsymbol{\xi},\, \boldsymbol{\xi}_*)$ of two colliding particles are changed into $(\boldsymbol{\xi}', \boldsymbol{\xi}'_*)$ in a collision process, is equal to the probability that $(\boldsymbol{\xi}', \boldsymbol{\xi}'_*)$ are changed into $(\boldsymbol{\xi},\, \boldsymbol{\xi}_*)$.

5. The Boltzmann chaos assumption: the velocities of two particles which are about to collide are uncorrelated. If two particles at position $\boldsymbol{x}$, which have not collided yet, are picked randomly, then the joint distribution of their velocities is given by the tensor product (in velocity space) of their one-particle functions.

Under these assumptions the one-particle function f satisfies the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \boldsymbol{x}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = Q(f, f), \tag{2.90}$$

where $\boldsymbol{F}$ is the macroscopic force acting the particles, and $Q(f, f)$ is the collision operator, which describes the influence of collisions between particles on the evolution of f.

If the considered system of particles is a mixture of n species, (2.90) changes into a system of n coupled Boltzmann equations for the n distribution functions f_j, $j = 1, ..., n$. In this case, the influence of collisions between particles of species j and k on f_j is described by n collision operators $Q_{jk}(f_j, f_k)$, $k = 1, ..., n$. Thus (2.90) becomes

$$\frac{\partial f_j}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f_j}{\partial \boldsymbol{x}} + \boldsymbol{F}_j \cdot \frac{\partial f_j}{\partial \boldsymbol{\xi}} = \sum_{k=1}^{n} Q_{jk}(f_j, f_k), \qquad j = 1, ..., n. \tag{2.91}$$

2.D.1 Connection to macroscopic quantities

From relations (2.90) or (2.91) one can derive equations for the evolution of the system of particles in terms of macroscopic quantities such as the physical density $\rho^{(j)}(\boldsymbol{x}, t)$, the momentum $(\rho\, \boldsymbol{v})^{(j)}(\boldsymbol{x}, t)$, and mass velocity $\boldsymbol{v}^{(j)}(\boldsymbol{x}, t)$ of the j-th species. The connection to the one-particle function is given by

$$\rho^{(j)} = \int_{\mathbb{R}^N} f_j \,\mathrm{d}\boldsymbol{\xi}, \qquad (\rho\, \boldsymbol{v})^{(j)} = \int_{\mathbb{R}^N} \boldsymbol{\xi}\, f_j \,\mathrm{d}\boldsymbol{\xi}, \qquad \boldsymbol{v}^{(j)} = \frac{(\rho\, \boldsymbol{v})^{(j)}}{\rho^{(j)}}.$$

The equations for the macroscopic quantities are obtained by multiplying the Boltzmann equation for the one-particle distribution (2.90) or (2.91) with a collision invariant ψ_α and integration over all possible velocities.

Single species. In the case of single species the index or superscript j is omitted. A function ψ is called a collision invariant if

$$\int_{\mathbb{R}^N} \psi\, Q(f, f) \,\mathrm{d}\boldsymbol{\xi} = 0.$$

The space of collision invariants is spanned by the five elementary collision invariants $\psi_0 =$ const, $(\psi_1, \psi_2, \psi_3) = \boldsymbol{\xi}$, $\psi_4 = |\boldsymbol{\xi}|^2$. The collision invariant ψ_0 corresponds to the conservation of mass, (ψ_1, ψ_2, ψ_3) to the conservation of momentum, and ψ_4 to the conservation of energy. Since we do not consider the energy equation, ψ_4 is neglected.

In the following, assume that the macroscopic force $\boldsymbol{F}$ is independent of $\boldsymbol{\xi}$ and $f(\boldsymbol{x},\, \boldsymbol{\xi},\, t) \to 0$ for $|\boldsymbol{x}| \to \infty$. Then, multiplying (2.90) by ψ_α, $\alpha = 1, \ldots, 4$, and integrating with respect to $\boldsymbol{\xi}$ yield the following equations for the macroscopic quantities (summation over repeated indices):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho\, v_i) &= 0, & \alpha &= 0, \\ \frac{\partial}{\partial t}(\rho\, v_\alpha) + \frac{\partial}{\partial x_i}\big(\rho\, v_\alpha\, v_i + \Pi_{\alpha i}\big) &= \rho\, F_\alpha, & \alpha &= 1, 2, 3. \end{aligned} \tag{2.92}$$

In (2.92), $\alpha = 0$ corresponds to the continuity equation, and $\alpha = 1, 2, 3$ correspond to the equations of motion. To derive (2.92) from (2.90), introduce the peculiar velocity $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{v}$, and use the relations

$$\int_{\mathbb{R}^N} \frac{\partial f}{\partial x_i} \,\mathrm{d}\boldsymbol{\xi} = 0, \qquad \int_{\mathbb{R}^N} \xi_k \frac{\partial f}{\partial x_i} \,\mathrm{d}\boldsymbol{\xi} = -\rho\, \delta_{ik}$$

$$\int_{\mathbb{R}^N} \xi_\alpha\, \xi_i\, f \,\mathrm{d}\boldsymbol{\xi} = \rho\, v_\alpha\, v_i + \Pi_{\alpha i}, \qquad \Pi_{\alpha i} = \int_{\mathbb{R}^N} c_\alpha\, c_i\, f \,\mathrm{d}\boldsymbol{\xi}.$$

The content of the following remark on the structure of Π can be found in [12, II.6]

Remark 2.D.1. *In any macroscopic approach to fluid dynamics, one has to postulate, either on the basis of experiments or by plausible arguments, some phenomenological relations (the so-called "constitutive equations") between $\Pi_{\alpha i}$ on one hand and ρ, v_i on the other. One well known model is the Navier-Stokes-Fourier (or viscous and thermally conducting) fluid:*

$$\Pi = (p - \lambda \operatorname{div} \boldsymbol{v})\, \mathbb{I} - \mu \left(\nabla \boldsymbol{v} + [\nabla \boldsymbol{v}]^T\right),$$

where μ and λ are the viscosity coefficients.

Mixtures. In the case of a mixture of n species (without chemical reactions or phase transition, etc.), it holds

$$\int_{\mathbb{R}^N} \psi \sum_{k=1}^{n} Q_{jk}(f_j,\, f_k)\, \mathrm{d}\boldsymbol{\xi} = 0, \qquad j = 1, \ldots, n,$$

for $\psi = \mathrm{const.}$, which corresponds to the conservation of mass for the j-th species, and

$$\sum_j \int_{\mathbb{R}^N} \psi_j \sum_k Q_{jk}(f_j,\, f_k)\, \mathrm{d}\boldsymbol{\xi} = 0,$$

for $\psi_j = \mathrm{const.}$, $\psi_j = \xi_\alpha$, $\alpha = 1, 2, 3$ or $\psi_j = |\boldsymbol{\xi}|^2$ (conservation of the total mass, momentum and energy). Instead of (2.92), the macroscopic variables for mixtures satisfy a continuity equation for each species and the conservation of the global momentum:

$$\begin{aligned} &(\rho^{(j)})_t + \operatorname{div}\big(\rho^{(j)}\, \boldsymbol{v}^{(j)}\big) = 0, \qquad j = 1, \ldots, n, \\ &\sum_{j=1}^{n} \Big[\big(\rho^{(j)}\, \boldsymbol{v}^{(j)}\big)_t + \operatorname{div}\big(\rho^{(j)}\, \boldsymbol{v}^{(j)} \otimes \boldsymbol{v}^{(j)} + \Pi^{(j)}\big) - \boldsymbol{F}_j\, \rho^{(j)} \Big] = \boldsymbol{0}. \end{aligned} \tag{2.93}$$

3 Theoretical investigations

This chapter is the theoretical part of the thesis. It contains the obtained results on the existence, uniqueness, and regularity of weak solutions to the problems derived in Chapter 2.

The chapter is structured as follows: in Section 3.1, we summarize the required assumptions and theoretical results obtained. Section 3.2 contains a short description of methods used during the proofs, a comparison with known results from the literature, and the conventions used in the subsequent sections. The next two sections immediately deal with the statement of the theoretical results. Section 3.3 deals with the transport problem and Section 3.4 with the decoupled measurement problem. References and results from the literature are given in the appendix.

3.1 Summary of the chapter

In Section 3.3, the transport problem (2.2) is considered. We show the existence of a non-empty time interval such that (2.2) admits a unique weak solution under suitable assumptions on the initial and boundary data. For the flow variables $\boldsymbol{U}$ and p we will assume that the initial and boundary functions satisfy: $\boldsymbol{U}^0 \in H^1(\Omega)^N$, $p^0 \in H^1(\Omega)$ and $\boldsymbol{U}_b \in H^{3/2}(\partial\Omega)^N$. It is supposed that the initial function ρ^0 for the particle density is Lipschitz continuous with $\operatorname{supp}\rho^0$ being separated from the boundary by a positive distance. We assume that the domain Ω has $\mathcal{C}^2$ boundary. This is necessary to extend $\boldsymbol{U}_b$ to an $H^2(\Omega)^N$ function using the trace theorem in Sobolev-spaces (Theorem 3.E.2), and to use the basis $\{\boldsymbol{\psi}_j\}$ of $L^2(\Omega)^N$ and $H^1_0(\Omega)^N$ given by Lemma 3.G.4. Under these assumptions we show the existence and uniqueness of weak solutions on a non-empty time interval $(0, T)$, $T > 0$ that is determined by the data. See Theorem 3.3.1 for the precise formulation.

Section 3.4 is devoted to the decoupled measurement problem (2.4). This problem is decomposed into the flow problem (2.1) and the evolution of the (scaled) particle density (2.5).

The flow problem (2.1) is investigated in Section 3.4.1. The main result here is the existence and uniqueness of weak solutions in a non-empty time interval $(0, T)$, $T > 0$ that is determined by the data. To obtain this result, we assume that the data of the problem satisfy: $\boldsymbol{U}_b \in H^{3/2}(\partial\Omega)$, $\boldsymbol{U}^0 \in H^2(\Omega)^N$, $p^0 \in H^1(\Omega)$ and $\boldsymbol{f} \in H^1(0, T; L^2(\Omega)^N)$. The domain Ω is assumed to be of class $\mathcal{C}^2$ for the same reason as in the case of the transport problem. See Theorem 3.4.4 for the precise formulation.

The evolution of the particle density (2.5) is considered in Section 3.4.2. The main result here is the existence and uniqueness of weak solutions on arbitrary time intervals provided the velocity field is sufficiently regular. To obtain this result we assume that the initial particle density ρ^0 is a positive function from $L^\infty(\Omega) \cap H^1(\Omega)$, and the initial surface mass density η^0 is given by the relation $\eta^0 = H(\rho^0)$. For simplicity, we suppose that the mass flux $g\,|\boldsymbol{U}_b \cdot \boldsymbol{\nu}|$ of the particles through the inlet is constant in time and that g is bounded. To show the existence of weak solutions on a given time interval we need less regularity of the velocity field than obtained from the solution of the flow problem. To obtain the uniqueness of weak solutions we need the essential boundedness of the divergence of the velocity field. Such a regularity exceeds that obtained from the analysis of the flow problem. The precise result is formulated in Theorem 3.4.21. An important tool to prove this theorem is a special embedding in anisotropic Sobolev spaces, which was communicated to me by Pavel Krejčí, see Theorem 3.4.34.

The existence of weak solutions to the decoupled measurement problem in bounded $\mathcal{C}^2$ domains follows from the results on the flow problem and the evolution of the particle density. The solution is unique provided the divergence of the velocity field from the flow problem is essentially bounded.

3.2 Used methods and conventions

The flow problem (2.1) and the transport problem (2.2) will both be treated by fixed-point methods. Thereby, we consider an arbitrary function $\boldsymbol{W}$, substitute it into the continuity equations and the convective terms of the momentum equations, and then study the solution operator $G : \boldsymbol{W} \mapsto \boldsymbol{U}$, compare [3]. In the following, the problem of finding $\boldsymbol{U}$ for a given $\boldsymbol{W}$ is called auxiliary problem.

Note that a difficulty in the treatment of the equations of weakly compressible fluids is the lack of a suitable energy inequality. Thus, the methods for incompressible or strongly compressible fluids cannot be applied directly. To illustrate this, assume for the moment that $\boldsymbol{U}_b = \boldsymbol{0}$ and $\boldsymbol{f} = \boldsymbol{0}$, multiply the momentum equation of (2.1) by $\boldsymbol{U}$, integrate over Ω, and use the conservation of mass to obtain

$$\int_\Omega \left[\frac{1}{2} \frac{\partial}{\partial t} \left(\rho_0 \, |\boldsymbol{U}|^2 + \gamma p^2 \right) + |\nabla \boldsymbol{U}|^2 + |\operatorname{div} \boldsymbol{U}|^2 \right] \mathrm{d}\boldsymbol{x} = -\rho_0 \int_\Omega U_j \, \frac{\partial U_i}{\partial x_j} \, U_i \, \mathrm{d}\boldsymbol{x},$$

where summation over repeated indices is assumed. Since the right-hand side does not vanish, and it can not be estimated through the initial and boundary data the energy estimate can not be deduced directly. To work around this difficulty, Banach's fixed-point theorem will be used. Let us briefly summarize methods applied to the problems under investigation and sketch the relation to the existing literature.

The transport problem. In contrast to [3], this problem is formulated as a separate problem whose treatment is more rigorous. We enhance the fixed-point scheme of [3] and gain an explicit representation of the pressure and the particle density. The representation of the particle density can also be found in [56]. To show the solvability of the auxiliary problem, we will use Galerkin's method and ideas of [47]. Then, we show that G is a contraction on a certain function space, provided that T is small enough. Problem (2.2) is similar to the flow problem for strongly compressible media. This problem is studied, for example, in [17, 41, 47, 56].

The flow problem. Compared to [3], we modify the fixed-point scheme, and use Lemma 3.B.2 instead of conventional Gronwall's inequality. Due to the modification of the fixed-point scheme, additional assumptions on the pressure can be avoided, and the problem can be treated rigorously. The use of Lemma 3.B.2 enables us to show the unique solvability for arbitrary $H^2(\Omega)^N$ initial values for the velocity. To show the solvability of the auxiliary problem, Galerkin's method is used to derive estimates for the velocity and its time derivative. This procedure is also applied in [36] for the treatment of incompressible viscid fluids. The existence of a fixed-point is shown by proving that G is a contraction on a certain function space.

Other methods for Navier-Stokes equations are studied, for instance, in [18, 36, 38, 40, 60]. Clearly, this list is not complete. One can consult the references in [40] for an extensive overview of the literature.

We note that a problem similar to (2.1) is studied in [60, §8] as an approximation to the Navier-Stokes equations. There, the problem of deriving a priori estimates is solved by introducing the stabilization term $1/2\,(\mathrm{div}\boldsymbol{U})\,\boldsymbol{U}$ in the momentum equation of (2.1). More precisely, the following problem is considered:

$$\begin{aligned}
\epsilon\,(p_\epsilon)_t + \mathrm{div}\,\boldsymbol{u}_\epsilon &= 0 && \text{in } \Omega\times(0,T),\\
(\boldsymbol{u}_\epsilon)_t + (\boldsymbol{u}_\epsilon\cdot\nabla)\boldsymbol{u}_\epsilon + \frac{1}{2}\,\mathrm{div}\,(\boldsymbol{u})_\epsilon\,\boldsymbol{u}_\epsilon - \nu\,\Delta\boldsymbol{u}_\epsilon + \nabla p_\epsilon &= \boldsymbol{f} && \text{in } \Omega\times(0,T),\\
\boldsymbol{u}_\epsilon &= \boldsymbol{0} && \text{on } \partial\Omega\times(0,T),\\
\boldsymbol{u}_\epsilon = \boldsymbol{u}^0, \qquad p_\epsilon &= p^0 && \text{at } t=0,
\end{aligned} \tag{3.1}$$

instead of (2.1). In (3.1), ν denotes the kinematic viscosity of the fluid. Multiplying the momentum equation in (3.1) by $\boldsymbol{u}_\epsilon$ and integrating over Ω yields

$$\int_\Omega \left[\frac{1}{2}\frac{\partial}{\partial t}\left(|\boldsymbol{u}_\epsilon|^2 + \epsilon\,p_\epsilon^2\right) + \nu|\nabla\boldsymbol{u}_\epsilon|^2\right]\mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{f}\cdot\boldsymbol{u}\,\mathrm{d}\boldsymbol{x}, \tag{3.2}$$

for sufficiently regular $\boldsymbol{u}_\epsilon$ and p_ϵ. Relation (3.2) is suitable to derive a priori estimates. Moreover, as $\epsilon\to 0$, a subsequence $(\boldsymbol{u}_{\epsilon'},\,p_{\epsilon'})$ of solutions of (3.1) converges to some solution $(\boldsymbol{u},\,p)$ of Navier-Stokes equations, see [60, Theorems 8.3 and 8.4] for the precise formulation. However, we are not interested in the limit $\gamma\to 0$ in problem (2.1). Therefore, fixed-point techniques are used in Section 3.4.1 to investigate the flow problem (2.1)

The evolution of the particle density. To investigate problem (2.5), the same method as in [4] (Rothe's method) is used. Here, the boundary condition on the inlet is changed to the Robin type condition, and the assumption of divergence-free velocity field is dropped. Due to the modification of the inlet condition, the estimations can be carried out without further assumptions on the trace of the solution. A priori estimates are similar to [4] but without assuming that the velocity field is divergence-free. To establish the required relation between the trace of the particle density and the surface mass density of adhered particles on the active part, we first apply results of Savaré on elliptic problems in Lipschitz domains to obtain additional regularity of the particle density. Then, we apply a special embedding theorem to obtain continuity properties of the particle density in time. The uniqueness follows then from Hilpert's inequality.

We use the following conventions. The terms Young's, Hölder's or Minkowski's inequalities are used in the usual way (see Theorems 3.A.1 – 3.A.4). Further, the results of Section 3.D are used without direct referring to this section. In the following, Ω is assumed to be a bounded domain in $\mathbb{R}^N$, $N\in\{2,3\}$, and Sobolev embeddings will mainly be applied in three dimensions because this is the most interesting case. The constants occurring thereby will be denoted by C_Ω to indicate the dependence on the domain.

3.3 The transport problem

This section is devoted to the theoretical investigation of the transport problem (2.2). For the theoretical investigation of (2.2), the system is transformed to homogeneous boundary conditions for the velocity. To simplify the notation, extend $\boldsymbol{U}_b$ to Ω by solving the following elliptic boundary-value problem:

$$\begin{aligned} -\mu\Delta\boldsymbol{\psi} - \xi\nabla\mathrm{div}\,\boldsymbol{\psi} &= \boldsymbol{0} \quad \text{in } \Omega, \\ \boldsymbol{\psi}|_{\partial\Omega} &= \boldsymbol{U}_b \quad \text{on } \partial\Omega. \end{aligned} \tag{3.3}$$

Then $\boldsymbol{U}_b \in H^2(\Omega)$ by Lemma 3.G.3, and (2.2) can be rewritten using $\boldsymbol{u} = \boldsymbol{U} - \boldsymbol{U}_b$ as follows:

$$\begin{aligned} \gamma p' + \mathrm{div}\,(\boldsymbol{u} + \boldsymbol{U}_b) &= 0, \\ (\rho^{(0)})_t + \mathrm{div}\big(\rho^{(0)}[\boldsymbol{u}^* + {\boldsymbol{U}_b}^*]\big) &= 0, \\ \big(\rho_0 + \rho^{(0)}\big)\big(\boldsymbol{u}_t + ([\boldsymbol{u} + \boldsymbol{U}_b]\cdot\nabla)\,[\boldsymbol{u} + \boldsymbol{U}_b]\big)& \\ +\nabla p - \mu\Delta\boldsymbol{u} - \xi\nabla\mathrm{div}\,\boldsymbol{u} &= \boldsymbol{f}, \\ \boldsymbol{u}|_{\partial\Omega} &= \boldsymbol{0}, \\ \boldsymbol{u}(\boldsymbol{x},0) = \boldsymbol{U}^0(\boldsymbol{x}) - \boldsymbol{U}_b, \quad p(\boldsymbol{x},0) = p^0(\boldsymbol{x}), \quad \rho^{(0)}&(\boldsymbol{x},0) = \rho^0(\boldsymbol{x}). \end{aligned} \tag{3.4}$$

Definition 3.3.1 (Weak solutions)**.** *Let $q > N$ be given, and let the space $W^{1,1}_{q,\infty}(\Omega \times (0,T))$ be defined as in Section 3.H. A triple of functions $(\boldsymbol{u},\, p,\, \rho^{(0)})$ with $\boldsymbol{u} \in H^1(0,T;L^2(\Omega)^N) \cap L^2(0,T;H^1_0(\Omega)^N)$, $p \in H^1(0,T;L^2(\Omega))$, and $\rho^{(0)} \in W^{1,1}_{q,\infty}(\Omega \times (0,T))$ is called weak solution of* (3.4)*, if the initial conditions are satisfied, and all of the following equations*

$$\begin{aligned} 0 &= \int_0^T \int_\Omega \Big[\big(\rho^{(0)}\big)_t + \mathrm{div}\big(\rho^{(0)}[\boldsymbol{u}^* + {\boldsymbol{U}_b}^*]\big)\Big]\,\psi_1 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t, \\ 0 &= \int_0^T \int_\Omega \big[\gamma\, p_t + \mathrm{div}\,(\boldsymbol{U}_b + \boldsymbol{u})\big]\cdot\psi_2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \\ 0 &= \int_0^T \int_\Omega \Big[\big(\rho_0 + \rho^{(0)}\big)\big(\boldsymbol{u}_t + ([\boldsymbol{u} + \boldsymbol{U}_b]\cdot\nabla)\,[\boldsymbol{u} + \boldsymbol{U}_b]\big) - \boldsymbol{f}\Big]\,\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \\ &\quad + \int_0^T \int_\Omega \left[\mu\,\nabla\boldsymbol{u} : \nabla\boldsymbol{\psi} + \xi\,\mathrm{div}\,(\boldsymbol{u})\,\mathrm{div}\,(\boldsymbol{\psi}) - p\,\mathrm{div}\,(\boldsymbol{\psi})\right]\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \end{aligned} \tag{3.5}$$

are fulfilled for all $\psi_1 \in L^1(0,T;L^{q'}(\Omega))$, $\psi_2 \in L^2(0,T;L^2(\Omega))$, and $\boldsymbol{\psi} \in L^2(0,T;H^1_0(\Omega)^N)$ where $1/q + 1/q' = 1$.

Note that the particles cannot leave Ω through the walls $\partial\Omega \setminus (\Gamma^{\mathrm{in}} \cup \Gamma^{\mathrm{out}})$. But if the velocity is regularized, it could happen that $\boldsymbol{U}^* \cdot \boldsymbol{\nu} \neq 0$ on $\partial\Omega \setminus (\Gamma^{\mathrm{in}} \cup \Gamma^{\mathrm{out}})$. Therefore, we will require that the particles are located strictly inside Ω at $t = 0$ to estimate the time when they can reach the boundary.

Now, the main result of Section 3.3 can be stated.

Theorem 3.3.2 (Main result for the transport problem)**.** *Let Ω be a bounded domain in $\mathbb{R}^N$ with $\mathcal{C}^2$ boundary. Let σ_δ (see Section 2.4.4) be nonnegative and Lipschitz-continuous with $\int_{\mathbb{R}^N} \sigma_\delta = 1$ and $\mathrm{supp}\,\sigma_\delta \subset B_\delta(\boldsymbol{0})$ for some $\delta > 0$, where $B_\delta(\boldsymbol{0})$ is the ball with radius δ and center at the origin. Suppose $\boldsymbol{U}^0 \in H^1(\Omega)^N$, $\boldsymbol{U}_b \in H^2(\Omega)^N$, $p^0 \in H^1(\Omega)$ and $\rho^0 \in \mathcal{C}^{0,1}(\Omega)$ with $\mathrm{dist}\big(\mathrm{supp}\,\rho^{(0)},\, \partial\Omega\big) \geq d > 0$ for some d.*

Then, there exists $T > 0$ such that (3.4) *has a unique weak solution $(\boldsymbol{u},\, p,\, \rho^{(0)})$ in $\Omega \times (0, T)$, provided that $\boldsymbol{f} \in L^2(0, T; L^2(\Omega)^N)$. The components of the solution belong to the spaces:*

$$\begin{aligned}\boldsymbol{u} &\in H^1(0, T; L^2(\Omega)^N) \cap L^\infty(0, T; H_0^1(\Omega)^N) \cap L^2(0, T; H^2(\Omega)^N),\\ p &\in H^1(0, T; H^1(\Omega)),\\ \rho^{(0)} &\in \mathcal{C}^{0,1}(\Omega \times (0, T)).\end{aligned}$$

Additionally it holds $\operatorname{supp} \rho^{(0)}(t) \subset \Omega$ *for $t \in [0, T]$. Remember that the velocity $\boldsymbol{U}$ is given by $\boldsymbol{U} = \boldsymbol{U}_b + \boldsymbol{u}$.*

Remark 3.3.3. *Using embedding theorems, one can deduce from Theorem 3.3.2:*

$$\begin{aligned}\boldsymbol{U} &\in \mathcal{C}([0, T]; H^{1-\epsilon}(\Omega)^N) \qquad \text{for } \epsilon > 0,\\ p &\in \mathcal{C}([0, T]; H^1(\Omega)).\end{aligned}$$

The next definition introduces functional spaces where we are looking for the functions $\boldsymbol{U}$ and $\boldsymbol{u}$.

Definition 3.3.4. *Let $T \in (0, \infty)$ and Ω be an open subset of $\mathbb{R}^N$, $N \in \{2, 3\}$. Define the following Banach-spaces:*

$$\begin{aligned}V &:= V(0, T) := H^1(0, T; L^2(\Omega)^N) \cap L^\infty(0, T; H^1(\Omega)^N) \cap L^2(0, T; H^2(\Omega)^N),\\ V_0 &:= V \cap L^\infty(0, T; H_0^1(\Omega)^N),\end{aligned}$$

endowed with the norms

$$\begin{aligned}\|\boldsymbol{U}\|_V &:= \|\boldsymbol{U}\|_{H^1(0,T;L^2(\Omega)^N)} + \|\boldsymbol{U}\|_{L^\infty(0,T;H_0^1(\Omega)^N)} + \|\boldsymbol{U}\|_{L^2(0,T;H^2(\Omega))}\,,\\ \|\boldsymbol{u}\|_{V_0} &:= \|\boldsymbol{u}\|_{H^1(0,T;L^2(\Omega)^N)} + \|\boldsymbol{u}\|_{L^\infty(0,T;H_0^1(\Omega)^N)} + \|\boldsymbol{u}\|_{L^2(0,T;H^2(\Omega))}\,.\end{aligned}$$

The proof of Theorem 3.3.2 is structured as follows. In Section 3.3.1, the auxiliary problem is formulated and representations of the pressure and the particle density are given. The right-hand side of the auxiliary problem is investigated in Section 3.3.2. In Section 3.3.3, the solvability of the auxiliary problem is considered. Finally, in Section 3.3.4 the proof of Theorem 3.3.2 is completed by showing the existence of a fixed-point in the auxiliary problem.

3.3.1 Representation of the pressure and the particle density

To obtain a fixed-point scheme for $\boldsymbol{u}$, introduce an arbitrary function $\boldsymbol{w}$ and replace $\boldsymbol{u}$ by $\boldsymbol{w}$ in the mass conservations and the nonlinear term of the momentum equation in (3.4). Then, the auxiliary problem reads:

$$\begin{aligned}\gamma\, p_t + \operatorname{div}(\boldsymbol{w} + \boldsymbol{U}_b) &= 0,\\ \big(\rho^{(0)}\big)_t + \operatorname{div}\big(\rho^{(0)}[\boldsymbol{w}^* + \boldsymbol{U}_b{}^*]\big) &= 0,\\ \big(\rho_0 + \rho^{(0)}\big)\boldsymbol{u}_t - \mu\Delta\boldsymbol{u} - \xi\nabla\operatorname{div}(\boldsymbol{u}) &= \boldsymbol{F}, \qquad (3.6)\\ \boldsymbol{u}|_{\partial\Omega} &= \boldsymbol{0},\\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{U}^0(\boldsymbol{x}) - \boldsymbol{U}_b(\boldsymbol{x}), \quad p(\boldsymbol{x}, 0) = p^0(\boldsymbol{x}), \quad \rho^{(0)}&(\boldsymbol{x}, 0) = \rho^0(\boldsymbol{x}).\end{aligned}$$

The right-hand side of the momentum equation in (3.6) is defined by

$$\boldsymbol{F} := \boldsymbol{F}(\boldsymbol{w}) := \boldsymbol{f} - \nabla p - \left(\rho_0 + \rho^{(0)}\right)\left([\boldsymbol{w} + \boldsymbol{U}_b] \cdot \nabla\right)[\boldsymbol{w} + \boldsymbol{U}_b]). \tag{3.7}$$

Note p and $\rho^{(0)}$ can be expressed in terms of $\boldsymbol{w}$, see equations (3.8) and (3.10) below. Therefore, $\boldsymbol{F}$ given by (3.7) can indeed be regarded as a mapping of $\boldsymbol{w}$. To show that (3.6) is solvable for $\boldsymbol{u}$, the regularity of the right-hand side (3.7) has to be investigated. To this end, we show first how the unknowns p and $\rho^{(0)}$ can be computed.

Assume $\boldsymbol{w} \in V_0$, then $\boldsymbol{U}_b \in H^2(\Omega)$ and the first equation in (3.6) show that p_t satisfies:

$$p_t = -\frac{1}{\gamma}\operatorname{div}(\boldsymbol{w} + \boldsymbol{U}_b) \qquad \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)).$$

Therefore, the pressure is given by

$$p(t) = p^0 - \frac{t}{\gamma}\operatorname{div}\boldsymbol{U}_b - \frac{1}{\gamma}\int_0^t \operatorname{div}\boldsymbol{w}(\tau)\,\mathrm{d}\tau \qquad \in H^1(0,T;H^1(\Omega)). \tag{3.8}$$

To obtain a formula for $\rho^{(0)}$, set $\boldsymbol{W} = \boldsymbol{w} + \boldsymbol{U}_b \in V$. Then $\rho^{(0)}$ is determined by the initial value problem

$$\begin{aligned} \rho_t^{(0)} + \operatorname{div}\bigl(\rho^{(0)}\,\boldsymbol{W}^*\bigr) &= 0 \quad \text{in } \Omega \times (0,T), \\ \rho^{(0)} &= \rho^0 \quad \text{for } t = 0. \end{aligned} \tag{3.9}$$

The regularized velocity field $\boldsymbol{W}^*$ satisfies the requirements of Theorem 3.H.1. Thus, the solution $\rho^{(0)}$ is given by the formula

$$\rho^{(0)}(\boldsymbol{x},t) = \rho^0\left(\boldsymbol{y}(0,t,\boldsymbol{x})\right) \cdot \exp\left(\int_0^t \operatorname{div}\left(\boldsymbol{W}^*(\boldsymbol{y}(\tau,t,\boldsymbol{x}),\,\tau)\right)\,\mathrm{d}\tau\right), \tag{3.10}$$

where $\boldsymbol{y}$ denote the characteristics of $\boldsymbol{W}^*$ (see (3.181)). Due to (3.10), the time when the particles reach the boundary can be estimated from below as follows. Using properties of convolutions, we get

$$\begin{aligned} \int_0^t \|\operatorname{div}\boldsymbol{W}^*(\tau)\|_{L^\infty(\Omega)}\,\mathrm{d}\tau &\le \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\int_0^t \|\operatorname{div}(\boldsymbol{W}(\tau))\|_{L^2(\Omega)}\,\mathrm{d}\tau \\ &\le T\,\|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\,\|\boldsymbol{W}\|_{L^\infty(0,T;H^1(\Omega)^N)} \end{aligned}$$

so that $\rho^{(0)}(\boldsymbol{x},t) \neq 0$ can occur only if $\boldsymbol{y}(\tau,\,t,\,\boldsymbol{x}) \in \operatorname{supp}\rho^0$ for some $\tau \in [0,t]$. By (3.181) and the embedding $H^{2-\epsilon}(\Omega) \subset \mathcal{C}(\overline{\Omega})$, it holds

$$|\boldsymbol{y}(\tau_1,\,t,\,\boldsymbol{x}) - \boldsymbol{y}(\tau_2,\,t,\,\boldsymbol{x})| \le C_\Omega\,T\,\|\boldsymbol{W}\|_{L^\infty(0,T;H^{2-\epsilon}(\Omega))}\,.$$

In order to ensure $\operatorname{supp}\rho^{(0)}(\cdot,t) \subset \Omega$, assume in the following that

$$T < \frac{d}{C_\Omega\,\|\boldsymbol{W}\|_{L^\infty(0,T;H^{2-\epsilon}(\Omega))}}$$

where d is the same number as in the hypothesis of Theorem 3.3.2. Additionally, $\rho^{(0)}$ is nonnegative and bounded due to (3.10). Applying Theorem 3.H.1 and setting

$$M_1 := \max\rho^0 \cdot \exp\left(\sqrt{N}\|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\,\|\boldsymbol{U}_b\|_{H^1(\Omega)^N}\right),$$

yields an upper bound for $\rho^{(0)}$ in terms of $\boldsymbol{w} = \boldsymbol{W} - \boldsymbol{U}_b$ as follows:

$$\rho_{\max} := M_1 \cdot \exp\left(T\sqrt{N}\|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\,\|\boldsymbol{w}\|_{L^\infty(0,T;H^1(\Omega)^N)}\right). \tag{3.11}$$

3.3.2 The convective term and the regularity of the right-hand side

In order to show the existence of weak solutions $\boldsymbol{u} \in V_0$ of (3.6), the regularity of $\boldsymbol{F}$ given by (3.7) has to be estimated. The following lemma specifies the regularity of the convective term.

Lemma 3.3.5. *Let $\boldsymbol{V}$, $\boldsymbol{W} \in V$ and $r \in L^\infty(\Omega \times (0,T))$ be arbitrary functions. Then there exists a constant C_V such that*

$$\|r \cdot (\boldsymbol{V} \cdot \nabla)\boldsymbol{W}\|^2_{L^2(0,T;L^2(\Omega)^N)} \leq C_V \sqrt{T}\, \|r\|^2_{L^\infty(\Omega\times(0,T))} \cdot \|\boldsymbol{V}\|^2_V \cdot \|\boldsymbol{W}\|^2_V.$$

The constant C_V is independent of $\boldsymbol{V}$, $\boldsymbol{W}$ and r.

Proof. Let v and w be arbitrary components of $\boldsymbol{V}$ and $\boldsymbol{W}$, respectively. Note that $r \cdot (\boldsymbol{V} \cdot \nabla)\boldsymbol{W}$ consists of a sum of terms of the form $r\, v\, w_{x_j}$. Therefore, it is enough to proof that

$$\begin{aligned}\left\|r\, v\, w_{x_j}\right\|^2_{L^2(0,t;L^2(\Omega))} \leq & C_\Omega \sqrt{t}\, \|r\|^2_{L^\infty(\Omega\times(0,T))} \cdot \\ & \cdot \|v\|^2_{L^\infty(0,t;H^1(\Omega))} \cdot \left\|w_{x_j}\right\|_{L^\infty(0,t;L^2(\Omega))} \cdot \left\|w_{x_j}\right\|_{L^2(0,t;H^1(\Omega))},\end{aligned}$$

for all $t \in (0,T)$, where C_Ω is independent of v, w and r. Obviously

$$\int_0^t \int_\Omega r^2\, v^2\, w^2_{x_j} \leq \|r\|^2_{L^\infty(\Omega\times(0,T))} \cdot \int_0^t \int_\Omega v^2 w^2_{x_j}.$$

Therefore, it remains to estimate the integrals on the right-hand side. To this end we will use Hölder's inequality with $p = 3$, $p' = 3/2$, the embeddings $H^1(\Omega) \subset L^6(\Omega)$, $H^{1/2}(\Omega) \subset L^3(\Omega)$, and the interpolation inequality $\|u\|^2_{H^{1/2}(\Omega)} \leq C_\Omega \|u\|_{H^1(\Omega)} \cdot \|u\|_{L^2(\Omega)}$ (see Theorem 3.E.7). We have

$$\begin{aligned}\int_0^t \int_\Omega v^2 w^2_{x_j} &\leq \int_0^t \|v\|^2_{L^6(\Omega)} \left\|w_{x_j}\right\|^2_{L^3(\Omega)} \leq C_\Omega \int_0^t \|v\|^2_{H^1(\Omega)} \left\|w_{x_j}\right\|^2_{H^{1/2}(\Omega)} \\ &\leq C_\Omega \|v\|^2_{L^\infty(0,t;H^1(\Omega))} \int_0^t \left\|w_{x_j}\right\|_{H^1(\Omega)} \left\|w_{x_j}\right\|_{L^2(\Omega)} \\ &\leq C_\Omega \|v\|^2_{L^\infty(0,t;H^1(\Omega))} \cdot \left\|w_{x_j}\right\|_{L^\infty(0,t;L^2(\Omega))} \cdot \left\|w_{x_j}\right\|_{L^2(0,T;H^1(\Omega))} \cdot \sqrt{t}.\end{aligned}$$

The last step is due to the application of Hölder's inequality. □

Now it is possible to show that $\boldsymbol{F}$ is square summable.

Lemma 3.3.6. *Assume $0 < T < \infty$, $\boldsymbol{f} \in L^2(0,T;L^2(\Omega)^N)$, and $\boldsymbol{W} \in V$. Define the function*

$$g : [0,\infty)^2 \to [0,\infty), \quad g(r,T) = r^2\, T^2 + T^{1/2}\, r^4 \cdot \exp\left(N^{1/2} \|\sigma_\delta\|_{L^2(\mathbb{R}^N)} T\, r\right).$$

Then $\boldsymbol{F}$ defined by (3.7) *can be estimated as follows:*

$$\|\boldsymbol{F}\|^2_{L^2(0,T;L^2(\Omega)^N)} \leq B_F(T) \cdot (1 + g\,(\|\boldsymbol{W}\|_V, T)).$$

The function B_F is non-decreasing in T and independent of $\boldsymbol{W}$.

Proof. By (3.8) and Hölder's inequality, it holds

$$\begin{aligned} \int_0^T \int_\Omega |\nabla p|^2 \mathrm{d}\boldsymbol{x}\mathrm{d}t &\le 2T \left\|p^0\right\|^2_{H^1(\Omega)} + \frac{2}{\gamma^2} \int_0^T \int_\Omega \left| \int_0^t \nabla \mathrm{div}\, \boldsymbol{W}(\tau)\, \mathrm{d}\tau \right|^2 \mathrm{d}\boldsymbol{x}\mathrm{d}t \\ &\le 2T \left\|p^0\right\|^2_{H^1(\Omega)} + \frac{2}{\gamma^2} \int_0^T \int_\Omega t \cdot \int_0^t \left|\nabla \mathrm{div}\, \boldsymbol{W}(\tau)\right|^2 \mathrm{d}\tau \mathrm{d}\boldsymbol{x}\mathrm{d}t \\ &\le 2T \left\|p^0\right\|^2_{H^1(\Omega)} + \frac{2T^2}{\gamma^2} \left\|\boldsymbol{W}\right\|^2_{L^2(0,T;H^2(\Omega)^N)} . \end{aligned} \tag{3.12}$$

The value $\rho_{\max}$ is bounded by

$$\rho_{\max} \le \max \rho^0 \cdot \exp\big(C\, T \left\|\boldsymbol{W}\right\|_V\big)$$

for $C > \sqrt{N} \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}$. Therefore

$$(\rho_0 + \rho_{\max}) \le \big(\rho_0 + \max \rho^0\big) \cdot \exp\big(C\, T \left\|\boldsymbol{W}\right\|_V\big). \tag{3.13}$$

Therefore Lemma 3.3.5, estimate (3.12), and definition (3.11) imply

$$\begin{aligned} \int_0^T \int_\Omega |\boldsymbol{F}|^2 \mathrm{d}\boldsymbol{x}\mathrm{d}t &\le C \int_0^T \int_\Omega \Big[|\boldsymbol{f}|^2 + |\nabla p|^2 + T^{1/2} \big(\rho_0 + \rho_{\max}\big)^2 \|\boldsymbol{W}\|_V^4 \Big] \\ &\le C \Big[\|\boldsymbol{f}\|^2_{L^2(0,T;L^2(\Omega)^N)} + T \left\|p^0\right\|^2_{H^1(\Omega)} + T^2 \|\boldsymbol{W}\|_V^2 + T^{1/2} \big(\rho_0 + \rho_{\max}\big)^2 \|\boldsymbol{W}\|_V^4 \Big], \end{aligned}$$

for C large enough. Using the bound (3.13) proves the lemma. □

3.3.3 Existence and uniqueness of solutions to the auxiliary problem

We turn to the solvability of the auxiliary problem (3.6). More precisely, we show that the following problem

$$\begin{aligned} \big(\rho_0 + \rho^{(0)}\big) \boldsymbol{u}_t - \mu \Delta \boldsymbol{u} - \xi \nabla \mathrm{div}\, \boldsymbol{u} &= \boldsymbol{F}, \\ \boldsymbol{u}|_{\partial\Omega} &= \boldsymbol{0}, \\ \boldsymbol{u}(\boldsymbol{x}, 0) &= \boldsymbol{U}^0(\boldsymbol{x}) - \boldsymbol{U}_b(\boldsymbol{x}) \end{aligned} \tag{3.14}$$

has a unique solution $\boldsymbol{u} \in V_0$ in the sense of Definition 3.3.7. Note that the $\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{w})$ (see (3.7)) and that p and $\rho^{(0)}$ are given by (3.8) and (3.10).

Definition 3.3.7. *An element $\boldsymbol{u} \in V_0$ is called a strong solution of* (3.14) *if the following equation*

$$\int_0^T \int_\Omega \Big[\big(\rho_0 + \rho^{(0)}\big) \boldsymbol{u}_t - \mu \Delta \boldsymbol{u} - \xi \nabla \mathrm{div}\, \boldsymbol{u} - \boldsymbol{F} \Big] \cdot \boldsymbol{\psi}\, \mathrm{d}\boldsymbol{x}\mathrm{d}t = 0, \tag{3.15}$$

holds true for all $\boldsymbol{\psi} \in L^2(0, T; H_0^1(\Omega)^N)$.

The goal of this section is to prove the following lemma.

Lemma 3.3.8. *Assume the hypothesis of Lemma 3.3.6. Then* (3.14) *has a unique strong solution $\boldsymbol{u} \in V_0$.*

Remark 3.3.9. *Due to the inclusions* $V_0 \subset H^1(0,T; L^2(\Omega)^N) \subset \mathcal{C}([0,T]; L^2(\Omega)^N)$*, the initial condition in* (3.14) *makes sense.*

The proof of Lemma 3.3.8 is divided into the following steps:

1. Construction of approximate solutions $\boldsymbol{u}^m$.
2. Estimation of $\boldsymbol{u}^m$ in several norms.
3. Show that a subsequence of $\{\boldsymbol{u}^m\}$ converges to a solution $\boldsymbol{u}$ of (3.14).

Step 1: construction of approximate solutions. The solution $\boldsymbol{u}$ of (3.14) is approximated via Faedo-Galerkin approximations. To construct them, we proceed similar to [47, Chapter 7].

Let $\{\boldsymbol{\psi}_j\}$, $\{\lambda_j\}$ be the sequences defined in Lemma 3.G.4. For $m \in \mathbb{N}$, define

$$X_m := \operatorname{span}\{\boldsymbol{\psi}_j\}_{j=1}^m \tag{3.16}$$

and construct the approximations $\boldsymbol{u}^m$ by the ansatz

$$\boldsymbol{u}^m(t,\boldsymbol{x}) = \sum_{k=1}^m a_k^m(t)\boldsymbol{\psi}_k(\boldsymbol{x}) \qquad m = 1, 2, ... \tag{3.17}$$

To obtain an equation for the coefficients a_j^m, replace $(\boldsymbol{u}, \boldsymbol{\psi})$ by $(\boldsymbol{u}^m, \boldsymbol{\psi}_j)$ in (3.15) and neglect the integral over $(0,T)$ to obtain

$$\int_\Omega \big(\rho_0 + \rho^{(0)}\big)\boldsymbol{u}_t^m(t) \cdot \boldsymbol{\psi}_j \,\mathrm{d}\boldsymbol{x} = \int_\Omega \left[\boldsymbol{F}(t) + \mu\Delta\boldsymbol{u}^m(t) + \xi\nabla\mathrm{div}\,\boldsymbol{u}^m(t)\right] \cdot \boldsymbol{\psi}_j \,\mathrm{d}\boldsymbol{x}. \tag{3.18}$$

By Lemma 3.G.4, the coefficients are determined by the system of ODEs

$$\sum_{k=1}^m \dot{a}_k^m(t) \cdot \int_\Omega \big(\rho_0 + \rho^{(0)}(t)\big)\boldsymbol{\psi}_k \cdot \boldsymbol{\psi}_j \,\mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{F}(t) \cdot \boldsymbol{\psi}_j \,\mathrm{d}\boldsymbol{x} - \lambda_j\, a_j^m(t), \qquad j = 1, ..., m,$$
$$a_j^m(0) = \int_\Omega \boldsymbol{u}^0 \cdot \boldsymbol{\psi}_j \,\mathrm{d}\boldsymbol{x}.$$

This can be written as an initial value problem for the vector $\boldsymbol{a}^m(t) = \big(a_1^m(t), ..., a_m^m(t)\big)^T$

$$M(t) \cdot \dot{\boldsymbol{a}}^m(t) = \boldsymbol{A}^m(\boldsymbol{a}^m(t)), \qquad a_j^m(0) = \int_\Omega \boldsymbol{u}^0 \cdot \boldsymbol{\psi}_j \,\mathrm{d}\boldsymbol{x},$$

where $A_j(\boldsymbol{a}^m) = \int_\Omega \boldsymbol{F} \cdot \boldsymbol{\psi}_j - \lambda_j\, a_j^m$ and the components of the matrix M are given by

$$M_{jk}(t) = \int_\Omega \rho_f(t)\boldsymbol{\psi}_j \cdot \boldsymbol{\psi}_k \,\mathrm{d}\boldsymbol{x}, \qquad \rho_f = \rho_0 + \rho^{(0)}.$$

Therefore, M is a symmetric matrix whose coefficients are real-valued and continuous in time because ρ_f is continuous. To see that (3.18) is solvable, we estimate the smallest and largest eigen-value of M. Define

$$\mathcal{M}_{\rho_f(t)} : X_m \to X_m, \quad \left\langle \mathcal{M}_{\rho_f(t)}\boldsymbol{v}\,;\,\boldsymbol{w}\right\rangle = \int_\Omega \rho_f(t)\boldsymbol{v} \cdot \boldsymbol{w}, \quad \boldsymbol{v}, \boldsymbol{w} \in X_m$$

Definition (3.11) implies that $\|\mathcal{M}_{\rho_f(t)}\|_{L(X_m,X_m)} \le \rho_0 + \rho_{\max}$ and the inequalities

$$\rho_0 \|\boldsymbol{v}\|^2_{L^2(\Omega)^N} \le \int_\Omega \rho_f(t)\boldsymbol{v}\cdot\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} \le (\rho_0+\rho_{\max})\,\|\boldsymbol{v}\|^2_{L^2(\Omega)^N}\,, \qquad \text{for all } \boldsymbol{v}\in X_m,$$

which show that the eigen-values of $M(t)$ lie in the interval $[\rho_0, \rho_0+\rho_{\max}] \subset (0,\infty)$. Thus, $M(t)$ is strictly positive, uniformly in t and m. Finally, $M(t)^{-1}$ exists and is continuous in time.

Therefore, (3.18) can be rewritten as

$$\boldsymbol{u}^m_t = \mathcal{M}^{-1}_{\rho_f(t)}\big(\boldsymbol{F}(t) + \mu\Delta\boldsymbol{u}^m(t) + \xi\nabla\mathrm{div}\,\boldsymbol{u}^m(t)\big),$$

and the theory of ODEs, shows the existence of $T_m > 0$ such that the solution $\boldsymbol{a}^m$ of

$$\dot{\boldsymbol{a}}^m(t) = M(t)^{-1}\boldsymbol{A}^m(\boldsymbol{a}^m(t)), \qquad a^m_j(0) = \int_\Omega \boldsymbol{u}^0\cdot\boldsymbol{\psi}_j\,\mathrm{d}\boldsymbol{x}, \qquad \text{for } j=1,...,m,$$

exists on $[0,T_m)$.

Step 2: a priori estimates on the approximate solutions. The solution of (3.14) will be obtained as a weak limit of the approximations $\boldsymbol{u}^m$. To this end, we show that they are bounded in V_0 independently of m.

Lemma 3.3.10. *Let the hypothesis of Lemma 3.3.6 be fulfilled for $T>0$. Then, for each $m\in\mathbb{N}$, the approximations $\boldsymbol{u}^m$ defined by* (3.17) *exist on $[0,T]$ and satisfy the estimate*

$$\|\boldsymbol{u}^m\|^2_{V_0} \le B_u(T)\cdot\big(1+g\big(T,\,\|\boldsymbol{W}\|_V\big)\big)\,.$$

The function B_u is non-decreasing in T and independent of $\boldsymbol{W}$ and m.

Proof. By construction of $\boldsymbol{u}^m$, the equation (3.18) remains valid if the basis function $\boldsymbol{\psi}_j$ is replaced by an arbitrary $\boldsymbol{\psi}\in X_m$. The idea of the proof is to choose first $\boldsymbol{\psi} = \boldsymbol{u}^m_t(t)$ and then $\boldsymbol{\psi} = [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^m(t)$. The choice $\boldsymbol{\psi} = \boldsymbol{u}^m_t$ yields after integration over $(0,t)$, $0<t<T_m$, and application of Young's inequality:

$$\begin{aligned}\int_\Omega \left[\frac{\mu}{2}|\nabla\boldsymbol{u}^m(t)|^2 + \frac{\xi}{2}|\mathrm{div}\,\boldsymbol{u}^m(t)|^2\right] + \int_0^t\int_\Omega \Big(\frac{\rho_0}{2}+\rho^{(0)}\Big)\,|\boldsymbol{u}^m_t|^2 \\ \le \int_\Omega \left[\frac{\mu}{2}|\nabla\boldsymbol{u}^0(t)|^2 + \frac{\xi}{2}|\mathrm{div}\,\boldsymbol{u}^0(t)|^2\right] + \int_0^t\int_\Omega \frac{1}{2\rho_0}|\boldsymbol{F}|^2.\end{aligned} \tag{3.19}$$

In the same way, $\boldsymbol{\psi} = [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^m$ yields

$$\int_0^t\int_\Omega \left|\frac{1}{2}\left[-\mu\Delta - \xi\nabla\mathrm{div}\right]\boldsymbol{u}^m\right|^2 \le \int_0^t\int_\Omega \Big[|\boldsymbol{F}|^2 + \big(\rho_0+\rho_{\max}\big)^2|\boldsymbol{u}^m_t|^2\Big]\,. \tag{3.20}$$

Multiply (3.20) by $(\rho_0/4)\cdot(\rho_0+\rho_{\max})^{-2}$ and add it to (3.19) to obtain:

$$\begin{aligned}\int_\Omega |\nabla\boldsymbol{u}^m(t)|^2 + \int_0^t\int_\Omega \Big[|\boldsymbol{u}^m_t|^2 + |[-\mu\Delta - \xi\nabla\mathrm{div}]\,\boldsymbol{u}^m|^2\Big] \\ \le C\left[\big\|\boldsymbol{u}^0\big\|^2_{H^1(\Omega)^N} + \|\boldsymbol{F}\|^2_{L^2(0,t;L^2(\Omega)^N)}\right],\end{aligned} \tag{3.21}$$

where C is sufficiently large.

Now, use Poincaré's inequality and the orthonormality of $\{\boldsymbol{\psi}_j\}$ in $L^2(\Omega)^N$ to obtain the bound

$$|\boldsymbol{a}^m(t)|^2 \le \|\boldsymbol{u}^m(t)\|^2_{L^2(\Omega)^N} \le C_\Omega \|\nabla \boldsymbol{u}^m(t)\|^2_{L^2(\Omega)^{N\times N}} \\ \le C\left[\left\|\boldsymbol{u}^0\right\|^2_{H^1(\Omega)^N} + \|\boldsymbol{F}\|^2_{L^2(0,t;L^2(\Omega)^N)}\right],$$

which shows that $\boldsymbol{a}^m$ exists and is bounded on $[0,T]$ whenever $\boldsymbol{F}$ is square summable over $[0,T]$. Since $[-\mu\Delta - \xi\nabla\mathrm{div}]$ is strongly elliptic, the definition of the norm in V_0 (see 3.3.4) and Lemma 3.3.6 yield the estimate

$$\|\boldsymbol{u}^m\|^2_{V_0} \le C\left[\left\|\boldsymbol{u}^0\right\|^2_{H^1(\Omega)^N} + B_F(T)\big(1 + g(T, \|\boldsymbol{W}\|_V)\right].$$

This proves the lemma. □

Step 3: passage to the limit. Due to the uniform bound given by Lemma 3.3.10 there exist an element $\boldsymbol{u} \in V_0$ such that a subsequence of $\{\boldsymbol{u}^m\}_{m\in\mathbb{N}}$ denoted again by $\{\boldsymbol{u}^m\}_{m\in\mathbb{N}}$ converges in the following sense

$$\begin{aligned} \boldsymbol{u}^m &\rightharpoonup \boldsymbol{u} && \text{weakly in } H^1(0,\, T;\, L^2(\Omega)^N), \\ \boldsymbol{u}^m &\overset{*}{\rightharpoonup} \boldsymbol{u} && *\text{-weakly in } L^\infty(0,T;H^1_0(\Omega)^N), \\ \boldsymbol{u}^m &\rightharpoonup \boldsymbol{u} && \text{weakly in } L^2(0,T;H^2(\Omega)^N). \end{aligned} \tag{3.22}$$

The next step is to show that $\boldsymbol{u}$ satisfies (3.15).

Lemma 3.3.11. *The weak limit $\boldsymbol{u} \in V_0$ given by* (3.22) *is a unique strong solution of the auxiliary problem* (3.14) *in the sense of Definition 3.3.7.*

Proof. By the construction of approximate solutions, see (3.17) and (3.18), the functions $\boldsymbol{u}^m$ satisfy

$$\int_0^T \int_\Omega \left[\big(\rho_0 + \rho^{(0)}\big)\boldsymbol{u}^m_t + [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^m - \boldsymbol{F}\right]\cdot\boldsymbol{\psi} = 0 \quad \text{for all } \boldsymbol{\psi} \in L^2(0,T;X_m).$$

Due to the convergence (3.22), it holds

$$\int_0^T \int_\Omega \left[\big(\rho_0 + \rho^{(0)}\big)\boldsymbol{u}_t + [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u} - \boldsymbol{F}\right]\cdot\boldsymbol{\psi} = 0 \tag{3.23}$$

for all $\boldsymbol{\psi} \in L^2(0,T;X_m)$. Lemma 3.G.4 ensures that $\bigcup_{m\in\mathbb{N}} X_m$ is dense in $L^2(\Omega)^N$. Thus,

$$\bigcup_{m\in\mathbb{N}} L^2(0,T;X_m) \quad \text{is a dense subset of} \quad L^2(0,T;L^2(\Omega)^N).$$

Moreover, $\boldsymbol{u} \in V_0 \subset H^1(0,T;L^2(\Omega)^N) \cap L^2(0,T;H^2(\Omega)^N)$, and the bound defined in (3.11) imply that $\big(\rho_0 + \rho^{(0)}\big)\boldsymbol{u}_t + [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u} - \boldsymbol{F}$ is a continuous linear functional on $L^2(0,T;L^2(\Omega)^N)$. To show that, use Hölder's inequality to obtain

$$\left|\int_0^T \int_\Omega \left[\big(\rho_0 + \rho^{(0)}\big)\boldsymbol{u}_t + [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u} - \boldsymbol{F}\right]\cdot\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t\right| \\ \le C\left[\|\boldsymbol{u}\|_{V_0} + \|\boldsymbol{F}\|_{L^2(0,T;L^2(\Omega)^N)}\right]\cdot\|\boldsymbol{\psi}\|_{L^2(0,T;L^2(\Omega)^N)}. \tag{3.24}$$

By the relations (3.23) and (3.24) we get

$$\int_0^T \int_\Omega \Big[\big(\rho_0 + \rho^{(0)}\big) \boldsymbol{u}_t + [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u} - \boldsymbol{F} \Big] \cdot \boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = 0$$

for all $\boldsymbol{\psi} \in L^2(0,T;L^2(\Omega)^N)$. The uniqueness of $\boldsymbol{u}$ follows from the linearity of problem (3.14). □

3.3.4 Fixed-point method

Assume the hypothesis of Lemma 3.3.6. Due to Lemma 3.3.8, one can then consider the mapping $\boldsymbol{W} \mapsto \boldsymbol{u} : V \to V_0$ which maps $\boldsymbol{W}$ onto the solution of the initial-boundary value problem (3.14). Since $\boldsymbol{u}$ is a weak limit of the approximate solutions (3.17) it satisfies the bound of Lemma 3.3.10. Since $\boldsymbol{W} = \boldsymbol{U}_b + \boldsymbol{w} \in V$ for $\boldsymbol{w} \in V_0$, one can also consider the mapping $\boldsymbol{w} \mapsto \boldsymbol{u} : V_0 \to V_0$. Similar to Lemma 3.3.10, $\boldsymbol{u}$ is bounded by

$$\|\boldsymbol{u}\|_{V_0}^2 \le B_u \cdot \big(1 + g_0(T,\, \|\boldsymbol{w}\|_V)\big), \qquad g_0(T,\, \|\boldsymbol{w}\|_V) = g(T,\, \|\boldsymbol{U}_b + \boldsymbol{w}\|_V). \tag{3.25}$$

By the definition of g in Lemma 3.3.6, there exists an independent of $\boldsymbol{w}$ constant B_0 such that

$$\begin{aligned} g_0(T,\, \|\boldsymbol{w}\|_V) \le B_0 \Big[& T^2\, \|\boldsymbol{U}_b\|_{H^2(\Omega)^N}^2 \\ & + T^{1/2}\, \|\boldsymbol{U}_b\|_{H^2(\Omega)^N}^4 \cdot \exp\!\big(B_0\, T \left[\|\boldsymbol{U}_b\|_{H^2(\Omega)} + \|\boldsymbol{w}\|_{V_0}\right]\big) \\ & + T^2 \|\boldsymbol{w}\|_{V_0}^2 + T^{1/2} \|\boldsymbol{w}\|_{V_0}^4 \cdot \exp\!\big(B_0\, T \left[\|\boldsymbol{U}_b\|_{H^2(\Omega)} + \|\boldsymbol{w}\|_{V_0}\right]\big) \Big]. \end{aligned} \tag{3.26}$$

Definition 3.3.12. *Let $\boldsymbol{U}^0 \in H^1(\Omega)^N$, $\boldsymbol{U}_b \in H^2(\Omega)^N$, $p^0 \in H^1(\Omega)$, $\boldsymbol{f} \in L^2(0,T;L^2(\Omega)^N)$ for some $T > 0$ and $\boldsymbol{w} \in V_0$. Define the solution operator G by the relation*

$$G : V_0 \to V_0\,, \quad G(\boldsymbol{w}) = \boldsymbol{u},$$

where $\boldsymbol{u}$ is a unique solution claimed by Lemma 3.3.11.

To complete the proof of Theorem 3.3.2, we apply Banach's fixed-point theorem to show that G has a unique fixed-point for sufficiently small T. To this end, we will first find a set M that satisfies $G(M) \subset M$. Then, we will show that G is a contraction on M at least for small T. Define the following sets

$$M(T,r) := \big\{ \boldsymbol{u} \in V_0 \;:\; \boldsymbol{u}(0) = \boldsymbol{u}^0 \;\wedge\; \|\boldsymbol{u}\|_V \le r \big\}$$

for $T > 0$ and $r > \|\boldsymbol{u}^0\|_{H_0^1(\Omega)^N}$. Substituting (3.26) into (3.25) for a $\boldsymbol{w} \in M(T,r)$ with $r^2 > B_u$ and denoting $R := \|\boldsymbol{U}_b\|_V + r$ yield

$$\|\boldsymbol{u}\|_{V_0}^2 \le B_u + B_u\, B_0\, R^2\, T^{1/2} \Big[T^{3/2} + R^2 \exp\left(B_0\, T\, R\right) \Big] \le r^2, \tag{3.27}$$

if T is sufficiently small. In this case $G(M(T,r)) \subset M(T,r)$.

The next step is to find T and r such that G is contractive on $M(T,r)$.

Inequality for difference of two solutions. Choose $\boldsymbol{w}_i \in V_0$, $\boldsymbol{u}_i = G(\boldsymbol{w}_i)$ and use the following notations: $\boldsymbol{W}_i = \boldsymbol{w}_i + \boldsymbol{U}_b$, $\boldsymbol{U}_i = \boldsymbol{u}_i + \boldsymbol{U}_b$ for $i = 1, 2$, $\tilde{\boldsymbol{w}} = \boldsymbol{w}_1 - \boldsymbol{w}_2$, $\tilde{\boldsymbol{u}} = \boldsymbol{u}_1 - \boldsymbol{u}_2$, $\tilde{p} = p_1 - p_2$, and $\tilde{\rho} = \rho_1^{(0)} - \rho_2^{(0)}$. By (3.14), the difference $\tilde{\boldsymbol{u}}$ solves the following problem

$$
\begin{aligned}
\gamma \tilde{p}_t + \operatorname{div}(\tilde{\boldsymbol{u}}) &= 0, \\
\big(\rho_0 + \rho_2^{(0)}\big) \tilde{\boldsymbol{u}}_t - \mu \Delta \tilde{\boldsymbol{u}} - \xi \nabla \operatorname{div}(\tilde{\boldsymbol{u}}) &= \tilde{\boldsymbol{F}}, \\
\tilde{\boldsymbol{u}}(0, \boldsymbol{x}) = \boldsymbol{0}\,, \quad \tilde{\boldsymbol{u}}|_{\partial\Omega} &= \boldsymbol{0},
\end{aligned}
$$

where

$$
\tilde{\boldsymbol{F}} = \nabla \tilde{p} - \tilde{\rho}\, \boldsymbol{u}_{1,t} - \tilde{\rho}\, [(\boldsymbol{W}_1 \cdot \nabla) \boldsymbol{W}_1] - \big(\rho_0 + \rho_2^{(0)}\big)\, [(\boldsymbol{W}_1 \cdot \nabla) \tilde{\boldsymbol{w}} + (\tilde{\boldsymbol{w}} \cdot \nabla) \boldsymbol{W}_2]\,. \tag{3.28}
$$

To estimate $\|\tilde{\boldsymbol{u}}\|_V$ in terms of $\|\tilde{\boldsymbol{w}}\|_V$, the right-hand side $\tilde{\boldsymbol{F}}$ has to be estimated. To this end, we first estimate $\tilde{p}$ (see (3.29)) and $\tilde{\rho}$ (see Lemma 3.3.13)

Similar to (3.8), $\tilde{p}$ is given by the formula

$$
\tilde{p}(t) = -\frac{1}{\gamma} \int_0^t \operatorname{div} \tilde{\boldsymbol{w}}(\tau)\, \mathrm{d}\tau,
$$

and therefore, Hölder's inequality yields the estimate

$$
\|\nabla \tilde{p}\|^2_{L^2(\Omega)^N} = \frac{1}{\gamma} \int_\Omega \left| \int_0^t \nabla \operatorname{div} \tilde{\boldsymbol{w}}(\tau)\, \mathrm{d}\tau \right|^2 \mathrm{d}\boldsymbol{x} \le \frac{T}{\gamma}\, \|\tilde{\boldsymbol{w}}\|_{L^2(0,T;H^2(\Omega)^N)}\,. \tag{3.29}
$$

For $\tilde{\rho}$ one can show the following estimate.

Lemma 3.3.13. *Let d be defined as in Theorem 3.3.2, and ρ^0 be nonnegative and Lipschitz-continuous with the Lipschitz-constant L_ρ. Moreover, let $\boldsymbol{W}_i \in V$ be given and ρ_i be solutions of* (3.9) *corresponding to velocity fields $\boldsymbol{W}_i^*$, $i = 1, 2$, respectively. Set $\tilde{\rho} = \rho_1 - \rho_2$ and $\tilde{\boldsymbol{W}} = \boldsymbol{W}_1 - \boldsymbol{W}_2$. Then there exists a constant $\tilde{B}_\rho$ such that*

$$
\tilde{\rho}(\boldsymbol{x}, t) \le \tilde{B}_\rho \sqrt{T}\, \left\| \tilde{\boldsymbol{W}} \right\|_{L^2(0,T;H^{2-\epsilon}(\Omega)^N)}\,.
$$

The constant $\tilde{B}_\rho$ depends on σ_δ, ρ^0, and $\|\boldsymbol{W}_i\|_V$, but not on $\tilde{\boldsymbol{W}}$.

Proof. The proof is divided into two steps. First, the difference of the characteristics $\tilde{\boldsymbol{y}}$ is estimated, second, $\tilde{\rho}$ is estimated.

Step 1 (estimate of the characteristics). By the equations (3.181), the difference of the characteristics $\tilde{\boldsymbol{y}} = \boldsymbol{y}_1 - \boldsymbol{y}_2$ solves the initial value problem

$$
\frac{\partial \tilde{\boldsymbol{y}}_1}{\partial \tau}(\tau, t, \boldsymbol{x}) = \boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau, t, \boldsymbol{x}), \tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_2(\tau, t, \boldsymbol{x}), \tau)\,, \qquad \tilde{\boldsymbol{y}}(t, t, \boldsymbol{x}) = \boldsymbol{0}.
$$

Assume that t and $\boldsymbol{x}$ are fixed and omit them for brevity. The difference of the trajectories at time s can be estimated as follows:

$$
\begin{aligned}
|\tilde{\boldsymbol{y}}(s)| &\le \int_0^s |\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau), \tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_2(\tau), \tau)|\, \mathrm{d}\tau \\
&\le \int_0^s \Big[|\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau), \tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_1(\tau), \tau)| \\
&\quad + |\boldsymbol{W}_2^*(\boldsymbol{y}_1(\tau), \tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_2(\tau), \tau)| \Big] \mathrm{d}\tau.
\end{aligned} \tag{3.30}
$$

Due to the embedding $H^{2-\epsilon}(\Omega) \subset \mathcal{C}^0(\bar{\Omega})$ the first term on the right-hand side can be estimated as follows:

$$\int_0^s |\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau),\tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_1(\tau),\tau)| \leq C_\Omega \, \|\boldsymbol{W}_1^* - \boldsymbol{W}_2^*\|_{L^2(0,T;H^{2-\epsilon}(\Omega)^N)} \sqrt{s}. \tag{3.31}$$

The second term on the right-hand side of (3.30) can be estimated using the Lipschitz-continuity of σ_δ. Denote the Lipschitz-constant of σ_δ by L_σ. The following estimate holds

$$\begin{aligned}
&\int_0^s |\boldsymbol{W}_2^*(\boldsymbol{y}_1(\tau),\tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_2(\tau),\tau)| \\
&\quad \leq \int_0^s \int_{\mathbb{R}^N} |\sigma_\delta(\boldsymbol{y}_1(\tau) - \boldsymbol{z}) - \sigma_\delta(\boldsymbol{y}_2(\tau) - \boldsymbol{z})| \cdot |\boldsymbol{W}_2(\boldsymbol{z},\tau)| \, \mathrm{d}\boldsymbol{z} \, \mathrm{d}\tau \\
&\quad \leq \int_0^s \left[\sup_{\boldsymbol{y}\in\Omega} |\boldsymbol{W}_2(\boldsymbol{y},\tau)| \cdot \int_M |\sigma_\delta(\boldsymbol{y}_1(\tau) - \boldsymbol{z}) - \sigma_\delta(\boldsymbol{y}_2(\tau) - \boldsymbol{z})| \, \mathrm{d}\boldsymbol{z} \right] \mathrm{d}\tau \\
&\quad \leq 2|B_\delta| \, L_\sigma \int_0^s \|\boldsymbol{W}_2\|_{H^{2-\epsilon}(\Omega)^N} \, |\tilde{\boldsymbol{y}}(\tau)| \mathrm{d}\tau,
\end{aligned} \tag{3.32}$$

where $M = B_\delta(\boldsymbol{y}_1(\tau)) \cup B_\delta(\boldsymbol{y}_1(\tau))$, and $|B_\delta|$ is the volume of a ball with radius δ. Substituting (3.31) and (3.32) into (3.30) yields

$$|\tilde{\boldsymbol{y}}(s)| \leq C_\Omega \sqrt{s} \, \|\boldsymbol{W}_1^* - \boldsymbol{W}_2^*\|_{L^2(0,T;H^{2-\epsilon}(\Omega))} + 2|B_\delta| \, L_\sigma \int_0^s \|\boldsymbol{W}_2\|_{H^{2-\epsilon}(\Omega)^N} \, |\tilde{\boldsymbol{y}}(\tau)| \mathrm{d}\tau.$$

Thus, Gronwall's inequality implies

$$\begin{aligned}
&|\tilde{\boldsymbol{y}}| \leq B_y \sqrt{T} \, \|\boldsymbol{W}_1^* - \boldsymbol{W}_2^*\|_{L^2(0,T;H^{2-\epsilon}(\Omega))}, \\
&B_y := C_\Omega \exp\left(2\sqrt{T} \, |B_\delta| L_\sigma \, \|\boldsymbol{W}_2\|_{L^2(0,T;H^{2-\epsilon}(\Omega)^N)} \right).
\end{aligned} \tag{3.33}$$

Step 2 (estimate for the densities). Due to Theorem 3.H.1, the difference $\tilde{\rho} = \rho_1 - \rho_2$ of solutions of (3.9) can be expressed by

$$\begin{aligned}
\tilde{\rho}(\boldsymbol{x}, s) &= \left[\rho^0(\boldsymbol{y}_1(s)) - \rho^0(\boldsymbol{y}_2(s))\right] \exp\left(\int_0^s \operatorname{div}\left(\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau),\tau)\right) \, \mathrm{d}\tau \right) \\
&+ \rho^0(\boldsymbol{y}_2(s)) \left[\exp\left(\int_0^s \operatorname{div}\left(\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau),\tau)\right) \mathrm{d}\tau \right) \right. \\
&\left. - \exp\left(\int_0^s \operatorname{div}\left(\boldsymbol{W}_2^*(\boldsymbol{y}_2(\tau),\tau)\right) \mathrm{d}\tau \right) \right].
\end{aligned} \tag{3.34}$$

The first term on the right-hand side of (3.34) can be estimated using properties of convolutions, the Lipschitz-continuity of ρ^0, and the estimate (3.33). We have

$$\begin{aligned}
&\left[\rho^0(\boldsymbol{y}_1(s)) - \rho^0(\boldsymbol{y}_2(s))\right] \exp\left(\int_0^s \operatorname{div}\left(\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau),\tau)\right) \, \mathrm{d}\tau \right) \\
&\leq L_\rho \, B_y \sqrt{T} \, \|\boldsymbol{W}_1^* - \boldsymbol{W}_2^*\|_{L^2(0,T;H^{2-\epsilon}(\Omega))} \\
&\times \exp\left(\sqrt{s} \, \|\sigma_\delta\|_{L^2(\mathbb{R}^N)} \, \|\boldsymbol{W}_1\|_{L^2(0,T;H^1(\Omega)^N)} \right).
\end{aligned} \tag{3.35}$$

To estimate the brackets on the right-hand side of (3.34), note that $\left|\mathrm{e}^a - \mathrm{e}^b\right| \le \mathrm{e}^K \, |b-a|$ for real $a,\, b < K$, and set $r = \max\{\|\boldsymbol{W}_i\|_{L^1(0,T;H^1(\Omega)^N)} \;:\; i = 1,2\}$. Using the properties of convolutions again, one deduces the following estimate

$$
\begin{aligned}
&\exp\left(\int_0^s \operatorname{div}\left(\boldsymbol{W}_1^*(\boldsymbol{y}_1(\tau),\tau)\right) \mathrm{d}\tau\right) - \exp\left(\int_0^s \operatorname{div}\left(\boldsymbol{W}_2^*(\boldsymbol{y}_2(\tau),\tau)\right) \mathrm{d}\tau\right) \\
&\quad \le \exp\Big(r\, \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\Big) \times \\
&\qquad \left|\int_0^s \operatorname{div}\left(\boldsymbol{W}_1^*(\boldsymbol{y}_1,\tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_1,\tau) + \boldsymbol{W}_2^*(\boldsymbol{y}_1,\tau) - \boldsymbol{W}_2^*(\boldsymbol{y}_2,\tau)\right)\, \mathrm{d}\tau\right| \\
&\quad \le \exp\Big(r\, \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\Big) \cdot \Big[\|\sigma_\delta\|_{L^2(\mathbb{R}^N)} \|\boldsymbol{W}_1 - \boldsymbol{W}_2\|_{L^1(0,T;H^1(\Omega)^N)} + \\
&\qquad \left|\int_0^s \int_{\mathbb{R}^N} \sigma_\delta(\boldsymbol{y}_1 - \boldsymbol{z}) - \sigma_\delta(\boldsymbol{y}_2 - \boldsymbol{z}) \operatorname{div}\left(\boldsymbol{W}_2(\boldsymbol{z})\right)\, \mathrm{d}\boldsymbol{z}\mathrm{d}s\right|\Big] \\
&\quad \le \exp\Big(r\, \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\Big) \cdot \Big[\|\sigma_\delta\|_{L^2(\mathbb{R}^N)} \sqrt{T}\, \|\boldsymbol{W}_1 - \boldsymbol{W}_2\|_{L^2(0,T;H^1(\Omega)^N)} + \\
&\qquad L_\sigma\, B_y \sqrt{T}\, \|\boldsymbol{W}_1 - \boldsymbol{W}_2\|_{L^2(0,T;H^{2-\epsilon}(\Omega)^N)} \|\boldsymbol{W}_2\|_{L^1(0,T;H^1(\Omega)^N)}\Big]
\end{aligned}
\tag{3.36}
$$

Noting that $\|\boldsymbol{W}\|_{H^1(\Omega)^N} \le \|\boldsymbol{W}\|_{H^{2-\epsilon}(\Omega)^N}$ for small ϵ, using the abbreviation

$$
\begin{aligned}
\tilde{B}_\rho &:= L_\rho\, B_y \cdot \exp\Big(\sqrt{s}\, \|\sigma_\delta\|_{L^2(\mathbb{R}^N)} \|\boldsymbol{W}_1\|_{L^2(0,T;H^1(\Omega)^N)}\Big) + \\
&\quad + \rho_{\max} \exp\Big(r\, \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\Big) \cdot \big[\|\sigma_\delta\|_{L^2(\mathbb{R}^N)} + L_\sigma\, B_y\, \|\boldsymbol{W}_2\|_{L^1(0,T;H^1(\Omega)^N)}\big],
\end{aligned}
$$

and substituting (3.35) and (3.36) into (3.34) yield

$$
\tilde{\rho}(\boldsymbol{x},s) \le \tilde{B}_\rho \sqrt{T}\, \|\boldsymbol{W}_1 - \boldsymbol{W}_2\|_{L^2(0,T;H^{2-\epsilon}(\Omega)^N)}\;, \qquad \forall\, (\boldsymbol{x},\, s) \in \Omega \times (0,T),
$$

which completes the proof of the lemma. □

Due to (3.11), one can redefine the constant $\rho_{\max}$ as follows:

$$
\rho_i^{(0)}(\boldsymbol{x},t) \le M_1 \cdot \exp\Big(r\, T \sqrt{N} \|\sigma_\delta\|_{L^2(\mathbb{R}^N)}\Big) =: \rho_{\max}, \qquad i = 1,2.
$$

The next lemma gives an estimate of $\tilde{\boldsymbol{F}}$ defined by (3.28). Denote the constant in time extension of $\boldsymbol{U}_b$ again by $\boldsymbol{U}_b$.

Lemma 3.3.14. *Let $\boldsymbol{w}_i \in M(T,r)$, $i = 1,2$ and $R = \|\boldsymbol{U}_b\|_V + r$. Then there exists $\tilde{B}_F$ such that*

$$
\left\|\tilde{\boldsymbol{F}}\right\|^2_{L^2(0,T;L^2(\Omega)^N)} \le \tilde{B}_F(T,r)\, \sqrt{T}\, \|\tilde{\boldsymbol{w}}\|^2_{V_0}.
$$

The constant $\tilde{B}_F$ depends on T, r, and other data that are fixed. The constant $\tilde{B}_F$ is non-decreasing in T, r.

Proof. For $\|\boldsymbol{w}_i\|_V \le r$, it holds: $\|\boldsymbol{W}_i\|_V \le R$. Applying Lemma 3.3.5 to each term separately yields

$$\left\| \left(\rho_0 + \rho_2^{(0)}\right) \left[(\boldsymbol{W}_1 \cdot \nabla)\tilde{\boldsymbol{w}} + (\tilde{\boldsymbol{w}} \cdot \nabla)\boldsymbol{W}_2\right] \right\|^2_{L^2(0,T;L^2(\Omega)^N)} \le 2C_V \left(\rho_0 + \rho_{\max}\right)^2 \sqrt{T}\, R^2 \|\tilde{\boldsymbol{w}}\|^2_{V_0},$$

$$\|\tilde{\rho}\, [(\boldsymbol{W}_1 \cdot \nabla)\boldsymbol{W}_1]\|^2_{L^2(0,T;L^2(\Omega)^N)} \le C_V T^{1/2} R^4 \cdot \tilde{B}_\rho^2 T \|\tilde{\boldsymbol{w}}\|^2_{V_0}.$$

In the derivation of the last inequality, we have used Lemma 3.3.13 to estimate $\tilde{\rho}$. Using again Lemma 3.3.13 and estimate (3.27), we get

$$\|\tilde{\rho}\, \boldsymbol{u}_{1,t}\|^2_{L^2(0,T;L^2(\Omega)^N)} \le (r\, \tilde{B}_\rho)^2\, T\, \|\tilde{\boldsymbol{w}}\|^2_{V_0}.$$

Note that $\tilde{\boldsymbol{W}} = \tilde{\boldsymbol{w}}$, for $\boldsymbol{W}_i = \boldsymbol{U}_b + \boldsymbol{w}_i,\ i = 1, 2$. By (3.29), the gradient of the pressure can be estimated as follows:

$$\|\nabla \tilde{p}\|^2_{L^2(0,T;L^2(\Omega)^N)} \le \frac{T^2}{\gamma}\, \|\tilde{\boldsymbol{w}}\|^2_{V_0}.$$

Combining all prefactors into a single one completes the proof the lemma. □

The next lemma gives an estimate for $\|\tilde{\boldsymbol{u}}\|_V$ in terms of $\|\tilde{\boldsymbol{w}}\|_V$.

Lemma 3.3.15. *Let $r > B_u^{1/2}$ and $T > 0$ satisfy (3.27). Let $\boldsymbol{w}_i \in M(T, r)$, $i = 1, 2$ and $\boldsymbol{u}_i = G(\boldsymbol{w}_i)$, $\tilde{\boldsymbol{u}} = \boldsymbol{u}_1 - \boldsymbol{u}_2$, $\tilde{\boldsymbol{w}} = \boldsymbol{w}_1 - \boldsymbol{w}_2$. For every $\kappa \in (0, 1)$, there exists $T_* > 0$ such that*

$$\|\tilde{\boldsymbol{u}}\|^2_{V_0} \le \kappa\, \|\tilde{\boldsymbol{w}}\|^2_{V_0},$$

where $V_0 = V_0(0, T_*)$.

Proof. By (3.15), $\tilde{\boldsymbol{u}}$ satisfies the equation

$$\int_0^T \int_\Omega \left[\left(\rho_0 + \rho_2^{(0)}\right) \tilde{\boldsymbol{u}}_t + \left[-\mu\Delta - \xi \nabla \mathrm{div}\right] \tilde{\boldsymbol{u}} - \tilde{\boldsymbol{F}} \right] \cdot \boldsymbol{\psi} = 0 \quad \text{for all } \boldsymbol{\psi} \in L^2(0, T; L^2(\Omega)^N).$$

The same techniques as in the proof of Lemma 3.3.10 yield the inequality

$$\int_\Omega |\nabla \tilde{\boldsymbol{u}}(t)|^2 \,\mathrm{d}\boldsymbol{x} + \int_0^t \int_\Omega \left[|\tilde{\boldsymbol{u}}_t|^2 + |\Delta \tilde{\boldsymbol{u}}|^2 + |\nabla \mathrm{div}\, \tilde{\boldsymbol{u}}|^2 \right] \mathrm{d}\boldsymbol{x}\mathrm{d}\tau \le C \int_0^t \int_\Omega |\tilde{\boldsymbol{F}}|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau,$$

for all $t \in (0, T)$. By Definition 3.3.4, the left-hand side is equivalent to the norm of $\tilde{\boldsymbol{u}}$ in V_0, and by Lemma 3.3.14, the right-hand side can be estimated from above by $C\, \tilde{B}_F(T, r)\, t^{1/2}\, \|\boldsymbol{w}\|^2_{V_0}$. Choosing $\kappa \in (0, 1)$ and setting

$$T_* = \min \left\{ T,\ \left| \frac{\kappa}{C\, \tilde{B}_F(T, r)} \right|^2 \right\}$$

yields $\|\tilde{\boldsymbol{u}}\|_{V_0} \le \kappa \|\boldsymbol{w}\|_{V_0}$ in $V_0(0, T_*)$. □

Now we use Banach's fixed-point theorem to deduce, that the solution operator G defined in Definition 3.3.12 has a unique fixed-point $\boldsymbol{u} \in V_0(0, T_*)$. Compute the pressure p using the formula (3.8), and the particle density $\rho^{(0)}$ using the formula (3.10). Then $(\boldsymbol{u},\ p,\ \rho^{(0)})$ is the unique weak solution of problem (3.4) in the sense of Definition 3.3.1.

The proof of Theorem 3.3.2 is completed, and the consideration of the transport problem is finished. Next, the decoupled measurement problem will be investigated.

3.4 The decoupled measurement problem

This section is devoted to the investigation of system (2.4) describing the decoupled measurement problem. The problem is decoupled in the following sense. The quantities $\boldsymbol{U}$ and p describing the flow can be computed independently of the particle variables ρ and η by solving the flow problem (2.1) Using the velocity field $\boldsymbol{U}$, the particle variables ρ and η are determined by system (2.5) describing the evolution of the particle density. The main result of Section 3.4 is stated in Theorem 3.4.1. For the definition of weak solutions, see Definitions 3.4.2 and 3.4.19 below.

Theorem 3.4.1 (Main result for the decoupled measurement problem)**.** *Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with $\mathcal{C}^2$ boundary. Assume the data for the flow variables satisfy $\boldsymbol{U}^0 \in H^2(\Omega)^N$, $\boldsymbol{U}_b \in H^{3/2}(\partial\Omega)^N$, and $p^0 \in H^1(\Omega)$, and the data for the particle variables satisfy $\rho^0 \in H^1(\Omega) \cap L^\infty(\Omega)$, $\rho^0 \geq 0$, $\eta^0 = H(\rho^0)$ in Γ, and $g \in L^\infty(\Gamma^{\text{in}})$. Then there exists $T > 0$ such that problem* (2.4) *admits a weak solution, provided that $\boldsymbol{f} \in H^1(0,T;L^2(\Omega)^N)$. The components of the solution lie in the spaces*

$$
\begin{aligned}
\boldsymbol{U} &\in W^{1,\infty}(0,T;L^2(\Omega)^N) \cap H^1(0,T;H^1(\Omega)^N) \cap L^\infty(0,T;H^2(\Omega)^N),\\
p &\in W^{1,\infty}(0,T;H^1(\Omega)) \cap H^2(0,T;L^2(\Omega)),\\
\rho &\in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^{(3-\epsilon')/2}(\Omega)) \cap L^\infty(\Omega \times (0,T)),\\
\eta &\in H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{1/2}(\Gamma)),
\end{aligned}
$$

where $\epsilon' > 0$ is arbitrary. If the velocity field $\boldsymbol{U}$ obtained from the flow problem possesses the additional regularity: $\|\operatorname{div} \boldsymbol{U}(t)\|_{L^\infty(\Omega)} \leq C_U^*$ for almost all $t \in (0,T)$, where C_U^* is a constant, then the solution is unique.

Theorem 3.4.1 follows from the results on the flow problem (see Theorem 3.4.4) and the results on the evolution of the particle density (see Theorem 3.4.21). This section is structured as follows. The flow problem is considered in Section 3.4.1, and the evolution of the particle density is considered in Section 3.4.2.

For the flow problem, we first construct an auxiliary problem in Section 3.4.1.1. The regularity of solutions of the flow problem is considered in Sections 3.4.1.2 – 3.4.1.3 under certain assumptions on the data of the problem. The assumptions are verified in Section 3.4.1.4. The solvability of the flow problem is proved in 3.4.1.5. See Definition 3.4.2 and Theorem 3.4.4 for precise formulations.

For the evolution of the particle density, we construct approximate solutions in Section 3.4.2.1. A priori estimates for the approximate solutions are established in Section 3.4.2.2. Weak limits of the approximate solutions are considered in Section 3.4.2.3. The existence of weak solution is proved in Section 3.4.2.4. The uniqueness of the solution is considered in Section 3.4.2.5. A special anisotropic embedding theorem is proved in Section 3.4.2.6. The embedding is used in Section 3.4.2.4 to establish additional regularity of the weak solution. The precise formulation of the results for the evolution of the particle density is given in Definition 3.4.19 and Theorem 3.4.21. For the embedding, see Definition 3.4.33 and Theorem 3.4.34.

3.4.1 The flow problem

In this section, the flow problem (2.1) is considered. For theoretical investigations, the system is transformed to homogeneous boundary conditions for the velocity. Similar to Section 3.3, extend

$\boldsymbol{U}_b$ to an $H^2(\Omega)^N$-function by solving the boundary value problem (3.3). Using $\boldsymbol{u} = \boldsymbol{U} - \boldsymbol{U}_b$ the flow problem can be rewritten as follows:

$$\begin{aligned} p_t + \operatorname{div}(\boldsymbol{U}_b + \boldsymbol{u}) &= 0 \\ \rho_0 \boldsymbol{u}_t + \rho_0 \left([\boldsymbol{U}_b + \boldsymbol{u}] \cdot \nabla\right)[\boldsymbol{U}_b + \boldsymbol{u}] + \nabla p - \mu\Delta\boldsymbol{u} - \xi\nabla \operatorname{div} \boldsymbol{u} &= \boldsymbol{f} \\ \boldsymbol{u}|_{\partial\Omega} &= \boldsymbol{0} \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}^0 := \boldsymbol{U}^0(\boldsymbol{x}) - \boldsymbol{U}_b(\boldsymbol{x}), \quad p(\boldsymbol{x}, 0) &= p^0(\boldsymbol{x}). \end{aligned} \tag{3.37}$$

Definition 3.4.2 (Weak solutions)**.** *A pair of functions $(\boldsymbol{u}, p)$ with $p \in H^1(0,T; L^2(\Omega))$ and $\boldsymbol{u} \in L^2(0,T; H^1_0(\Omega)^N) \cap H^1(0,T; L^2(\Omega)^N)$ is called weak solution of* (3.37)*, if the initial conditions are satisfied and all of the following equations*

$$\int_0^T \int_\Omega [\gamma\, p_t + \operatorname{div}(\boldsymbol{U}_b + \boldsymbol{u})] \cdot \zeta \,\mathrm{d}\boldsymbol{x}\mathrm{d}t = 0,$$

$$\begin{aligned} &\int_0^T \int_\Omega \Big[\rho_0\, \boldsymbol{u}_t - \rho_0 \left([\boldsymbol{U}_b + \boldsymbol{u}] \cdot \nabla\right)[\boldsymbol{U}_b + \boldsymbol{u}] - \boldsymbol{f}\Big] \cdot \boldsymbol{\psi} \,\mathrm{d}\boldsymbol{x}\mathrm{d}t \\ + &\int_0^T \int_\Omega \Big[\mu\, \nabla\boldsymbol{u} : \nabla\boldsymbol{\psi} + \xi \operatorname{div}(\boldsymbol{u}) \operatorname{div}(\boldsymbol{\psi}) - p \operatorname{div}(\boldsymbol{\psi})\Big] \mathrm{d}\boldsymbol{x}\mathrm{d}t = 0 \end{aligned}$$

hold for all $\zeta \in L^2(0,T; L^2(\Omega))$, $\boldsymbol{\psi} \in L^2(0,T; H^1_0(\Omega)^N)$.

The next definition introduces functional spaces where we are looking for the functions $\boldsymbol{U}$ and $\boldsymbol{u}$.

Definition 3.4.3. *Let $T \in (0,\infty)$, Ω be an open subset of $\mathbb{R}^N$, $N \in \{2,3\}$. Define*

$$W := W(0,T) := \left\{ \boldsymbol{u} \in L^\infty(0,T; H^2(\Omega)^N) \;\middle|\; \begin{aligned} \boldsymbol{u}_t \in L^2(0,T; H^1(\Omega)^N) \\ \cap L^\infty(0,T; L^2(\Omega)^N) \end{aligned} \right\},$$

$$W_0 := W \cap L^\infty(0,T; H^1_0(\Omega)^N),$$

being endowed with the norms

$$\|\boldsymbol{U}\|^2_W := \|\boldsymbol{U}\|^2_{L^\infty(0,T;H^2(\Omega)^N)} + \|\boldsymbol{U}_t\|^2_{L^2(0,T;H^1(\Omega)^N)} + \|\boldsymbol{U}_t\|^2_{L^\infty(0,T;L^2(\Omega))},$$

$$\|\boldsymbol{u}\|^2_{W_0} := \|\boldsymbol{u}\|^2_{L^\infty(0,T;H^2(\Omega)^N)} + \|\boldsymbol{u}_t\|^2_{L^2(0,T;H^1_0(\Omega)^N)} + \|\boldsymbol{u}_t\|^2_{L^\infty(0,T;L^2(\Omega))}.$$

The main result of this section is stated in the following theorem.

Theorem 3.4.4 (Main result for the flow problem)**.** *Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with $\mathcal{C}^2$ boundary. Assume $\boldsymbol{U}_b \in H^{3/2}(\partial\Omega)$, $\boldsymbol{U}^0 \in H^2(\Omega)^N$ and $p^0 \in H^1(\Omega)$. Then there exists $T > 0$ such that the system* (3.37) *has a unique generalized weak solution in the sense of Definition 3.4.2. The functions $\mathbf{u}$ and p lie in the spaces*

$$\begin{aligned} &\boldsymbol{u} \in W_0, \\ &p \in W^{1,\infty}(0,T; H^1(\Omega)) \cap H^2(0,T; L^2(\Omega)), \end{aligned}$$

provided that $\boldsymbol{f} \in H^1(0,T; L^2(\Omega)^N)$. Remember that the velocity $\boldsymbol{U}$ is given by $\boldsymbol{U} = \boldsymbol{U}_b + \boldsymbol{u}$.

3.4.1.1 Construction of approximate solutions

Theorem 3.4.4 will be proved by a fixed-point technique. To obtain a fixed-point scheme for the velocity, proceed similar to Section 3.3.1. Introduce an arbitrary function $\boldsymbol{w}$ and replace $\boldsymbol{u}$ by $\boldsymbol{w}$ in the mass conservation equation and the convective term of the momentum equation. If $\boldsymbol{w} \in W_0$ is known, the pressure p satisfies the following relations (compare (3.8)):

$$\begin{aligned} p_t &= -\frac{1}{\gamma} \operatorname{div}(\boldsymbol{U}_b + \boldsymbol{w}) && \in L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T,L^2(\Omega)), \\ p(t) &= p^0 - \frac{1}{\gamma}\int_0^t \operatorname{div}(\boldsymbol{U}_b + \boldsymbol{w}(\tau))\, \mathrm{d}\tau && \in W^{1,\infty}(0,T;H^1(\Omega)) \cap H^2(0,T;L^2(\Omega)). \end{aligned} \tag{3.38}$$

Further, define the right-hand side $\boldsymbol{F}$ as follows

$$\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{w}) := \boldsymbol{f} + \nabla p - \rho_0 \left([\boldsymbol{w} + \boldsymbol{U}_b]\cdot\nabla\right)[\boldsymbol{w} + \boldsymbol{U}_b]\,. \tag{3.39}$$

For a given $\boldsymbol{w}$, problem (3.37) can be rewritten as the parabolic initial-boundary value problem

$$\begin{aligned} \rho_0 \boldsymbol{u}_t - \mu\Delta\boldsymbol{u} - \xi\nabla\operatorname{div}\boldsymbol{u} &= \boldsymbol{F} && \text{in } \Omega\times(0,T), \\ \boldsymbol{u} &= \boldsymbol{0} && \text{on } \partial\Omega\times(0,T), \\ \boldsymbol{u}(\boldsymbol{x},0) &= \boldsymbol{u}^0(\boldsymbol{x}) && \text{for } t = 0. \end{aligned} \tag{3.40}$$

Clearly, (3.40) has a unique weak solution $\boldsymbol{u}$ which satisfies the equation

$$\int_0^T \int_\Omega [\rho_0\, \boldsymbol{u}_t + [-\mu\,\Delta - \xi\,\nabla\mathrm{div}]\boldsymbol{u} - \boldsymbol{F}]\cdot\boldsymbol{\psi} = 0, \quad \forall\boldsymbol{\psi}\in L^2(0,T;L^2(\Omega)^N), \tag{3.41}$$

provided that $\boldsymbol{u}^0$ and $\boldsymbol{F}$ are sufficiently regular. The goal of the following construction is to show that $\boldsymbol{u}\in W_0$, if $\boldsymbol{w}\in W_0$ and $\boldsymbol{F}$ is computed as in the definition (3.39). In Lemma 3.4.12 below, we show that $\boldsymbol{w}\in W_0$ implies $\boldsymbol{F}\in H^1(0,T;L^2(\Omega)^N)$.

To show that $\boldsymbol{u}\in W_0$, we proceed similar to Section 3.3.3. Let $\{\lambda_j\}$ and $\{\boldsymbol{\psi}_j\}$ be the sequences defined in Lemma 3.G.4, define the spaces X_m as in (3.16), and consider the approximations $\boldsymbol{u}^m$ defined in (3.17). To obtain an equation for the coefficients, neglect the integral over $(0,T)$ in (3.41), and replace $(\boldsymbol{u},\,\boldsymbol{\psi})$ by $(\boldsymbol{u}^m,\,\boldsymbol{\psi}_j)$, $j = 1,\dots,m$ to obtain

$$\int_\Omega [\rho_0\, \boldsymbol{u}_t^m(t) + [-\mu\,\Delta - \xi\,\nabla\mathrm{div}]\boldsymbol{u}^m(t) - \boldsymbol{F}(t)]\cdot\boldsymbol{\psi}_j\,\mathrm{d}\boldsymbol{x} = 0, \qquad j = 1,\dots,m. \tag{3.42}$$

Then, the coefficients a_j^m of $\boldsymbol{u}^m$ are determined by the following initial value problem

$$\begin{aligned} \rho_0\, \dot a_j^m(t) + \lambda_j\, a_j^m(t) - \int_\Omega \boldsymbol{F}(t)\cdot\boldsymbol{\psi}_j\,\mathrm{d}\boldsymbol{x} &= 0, \\ a_j^m(0) &= \int_\Omega \boldsymbol{u}^0\cdot\boldsymbol{\psi}_j\,\mathrm{d}\boldsymbol{x} \qquad (j = 1,\dots,m). \end{aligned} \tag{3.43}$$

This system of ODEs can be written in matrix-vector notation as follows:

$$\rho_0\,\dot{\boldsymbol{a}}^m + \boldsymbol{A}^m(\boldsymbol{a}^m(t)) = \boldsymbol{0}, \qquad a_j^m(0) = \int_\Omega \boldsymbol{u}^0\cdot\boldsymbol{\psi}_j\,\mathrm{d}\boldsymbol{x}, \qquad (j = 1,\dots,m), \tag{3.44}$$

where the components A_j^m are given by $A_j^m(\boldsymbol{a}^m(t)) = \lambda_j\, a_j^m(t) - \int_\Omega \boldsymbol{F}(t)\cdot\boldsymbol{\psi}_j$. The theory of ODEs shows the existence of $T_m > 0$ such that the solution $\boldsymbol{a}^m$ exists on $[0,T_m)$.

3.4.1.2 A priori estimates

In this section, the approximations $\boldsymbol{u}^m$ defined in Section 3.4.1.1 are estimated in several norms. The method is similar to [36]. The following lemma shows that the approximations $\boldsymbol{u}^m$ exist on a certain non-empty time interval independent of m.

Lemma 3.4.5. *Let $\boldsymbol{u}^0 \in H_0^1(\Omega)^N$ and $\boldsymbol{F} \in L^2(0,T;L^2(\Omega)^N)$ for some $T > 0$. Then, for each m, the solutions $\boldsymbol{a}^m$ of* (3.44) *exist on $[0,T]$. Further there exists an independent of m constant B_1 such that the approximations $\boldsymbol{u}^m$ satisfy the estimates*

$$\left.\begin{array}{l} \|\boldsymbol{u}^m\|^2_{L^\infty(0,T;H_0^1(\Omega)^N)} \\ \|\boldsymbol{u}^m\|^2_{L^2(0,T;H^2(\Omega)^N)} \\ \|\boldsymbol{u}_t^m\|^2_{L^2(0,T;L^2(\Omega)^N)} \end{array}\right\} \leq B_1 \cdot \left[\|\boldsymbol{u}^0\|^2_{H_0^1(\Omega)^N} + \|\boldsymbol{F}\|^2_{L^2(0,T;L^2(\Omega)^N)}\right].$$

Proof. The idea of the proof is to replace the basis function $\boldsymbol{\psi}_j$ in (3.42) by $\boldsymbol{\psi}_j = \boldsymbol{u}_t^m(t)$ and by $\boldsymbol{\psi}_j = [-\mu\,\Delta - \xi\,\nabla\mathrm{div}]\boldsymbol{u}^m(t)$. To this end, fix $m \in \mathbb{N}$, multiply (3.43) by $\dot{a}_j^m(t)$, and sum up over $j \in \{1,...,m\}$. This is equivalent to replacing $\boldsymbol{\psi}_j$ by $\boldsymbol{u}_t^m$ in (3.42). After integrating the resulting equation over $(0,s)$, $s \in (0,T_m)$, and applying Young's inequality, we obtain

$$\begin{aligned} &\frac{\rho_0}{2}\int_0^s\int_\Omega |\boldsymbol{u}_t^m|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}t + \int_\Omega \left[\mu\,|\nabla\boldsymbol{u}^m(s)|^2 + \xi|\mathrm{div}\,\boldsymbol{u}^m(s)|^2\right]\mathrm{d}\boldsymbol{x} \\ &\quad\leq \int_\Omega \left[\mu\,|\nabla\boldsymbol{u}^0|^2 + \xi|\mathrm{div}\,\boldsymbol{u}^0|^2\right]\mathrm{d}\boldsymbol{x} + \int_0^s\int_\Omega \frac{1}{2\rho_0}|\boldsymbol{F}|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}t. \end{aligned} \tag{3.45}$$

To replace $\boldsymbol{\psi}_j$ by $[-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^m$, multiply (3.43) by $\lambda_j\, a_j^m(t)$ and sum up over $j \in \{1,...,m\}$ to obtain

$$\begin{aligned} &\frac{\rho_0}{2}\int_\Omega \left[\mu|\nabla\boldsymbol{u}^m(s)|^2 + \xi|\mathrm{div}\,\boldsymbol{u}^m(s)|^2\right]\mathrm{d}\boldsymbol{x} + \frac{1}{2}\int_0^s\int_\Omega |[-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^m|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau \\ &\quad\leq \frac{\rho_0}{2}\int_\Omega \left[\mu|\nabla\boldsymbol{u}^0|^2 + \xi|\mathrm{div}\,\boldsymbol{u}^0|^2\right]\mathrm{d}\boldsymbol{x} + \frac{1}{2}\int_0^s\int_\Omega |\boldsymbol{F}|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau. \end{aligned} \tag{3.46}$$

We show next that $\boldsymbol{a}^m$ exists on $[0,T]$. Using Poincare's inequality in (3.46) and the orthonormality of $\{\boldsymbol{\psi}_j\}$ in $L^2(\Omega)^N$, we obtain the following estimate

$$\begin{aligned} |\boldsymbol{a}^m(t)|^2 = \int_\Omega |\boldsymbol{u}^m(t)|^2\,\mathrm{d}\boldsymbol{x} &\leq C_P\int_\Omega |\nabla\boldsymbol{u}^m(t)|^2\,\mathrm{d}\boldsymbol{x} \\ &\leq C\left[\int_\Omega |\nabla\boldsymbol{u}^0|^2\,\mathrm{d}\boldsymbol{x} + \int_0^{T_m}\int_\Omega |\boldsymbol{F}|^2\mathrm{d}\boldsymbol{x}\mathrm{d}\tau\right], \end{aligned}$$

for all $t \in [0,T_m)$. For $T^m \leq T$, the right-hand side is bounded because $\boldsymbol{F} \in L^2(0,T;L^2(\Omega)^N)$. This implies that $\boldsymbol{a}^m$ exists on $[0,T]$.

Next, show the claimed estimates of $\boldsymbol{u}^m$. Combining (3.45) and (3.46) yields

$$\begin{aligned} &\int_\Omega |\nabla\boldsymbol{u}^m(t)|^2\,\mathrm{d}\boldsymbol{x} + \int_0^T\int_\Omega \left[|\boldsymbol{u}_t^m|^2 + \left|[-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^m\right|^2\right]\mathrm{d}\boldsymbol{x}\mathrm{d}\tau \\ &\quad\leq C\left[\|\boldsymbol{u}^0\|^2_{H_0^1(\Omega)^N} + \|\boldsymbol{F}\|^2_{L^2(0,T;L^2(\Omega)^N)}\right]. \end{aligned}$$

Noting that $-\mu\,\Delta - \xi\,\nabla\mathrm{div}$ is strongly elliptic proves the lemma (see Theorem 3.G.2). □

Let us derive additional estimates of $\boldsymbol{u}_t^m$. To this end, we assume in the following that $\boldsymbol{u}^0 \in H^2(\Omega)^N \cap H_0^1(\Omega)^N$ and $\boldsymbol{F} \in H^1(0,T;L^2(\Omega)^N)$. Due to (3.40), the time derivative $\boldsymbol{u}_t^m$ of $\boldsymbol{u}^m$ satisfies the following initial boundary value problem

$$\int_\Omega [\rho_0\, \boldsymbol{u}_{tt}^m + [-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}_t^m - \boldsymbol{F}_t] \cdot \boldsymbol{\psi}\, \mathrm{d}\boldsymbol{x}\mathrm{d}t = 0,$$
$$\boldsymbol{u}_t^m|_{\partial\Omega} = \mathbf{0},$$
$$\boldsymbol{u}_t^m(0) = P_{X_m}\left(\rho_0^{-1}[\mu\Delta + \xi\nabla\mathrm{div}]\boldsymbol{u}^0 + \boldsymbol{F}(0)\right),$$

where P_{X_m} denotes the orthogonal projection in $L^2(\Omega)^N$ onto X_m (see definition (3.16). Due to the construction (3.43), the coefficients $\dot{a}_j^m$ of $\boldsymbol{u}_t^m$ are solutions of the following initial value problem

$$\begin{aligned} &\rho_0\, \ddot{a}_j^m(t) + \lambda_j\, \dot{a}_j^m(t) - \int_\Omega \boldsymbol{F}(t)\cdot\boldsymbol{\psi}_j\, \mathrm{d}\boldsymbol{x} = 0, \\ &\dot{a}_j^m(0) = \frac{1}{\rho_0}\int_\Omega \boldsymbol{F}(0)\cdot\boldsymbol{\psi}_j\, \mathrm{d}\boldsymbol{x} - \frac{\lambda_j}{\rho_0}\, a_j^m(0), \qquad (j = 1, ..., m). \end{aligned} \tag{3.47}$$

Thus, system (3.47) can be rewritten as follows:

$$\begin{aligned} &\int_\Omega [(\rho_0\, \boldsymbol{u}_{tt}^m(t) - \boldsymbol{F}_t)\cdot\boldsymbol{\psi} + \mu\, \nabla\boldsymbol{u}_t^m(t) : \nabla\boldsymbol{\psi} + \xi\, \mathrm{div}\,(\boldsymbol{u}_t^m(t))\,\mathrm{div}\,(\boldsymbol{\psi})]\ \mathrm{d}\boldsymbol{x} = 0 \\ &\boldsymbol{u}_t^m(0) = P_{X_m}\left(\rho_0^{-1}\left[\boldsymbol{F}(0) + \mu\Delta\boldsymbol{u}^0 + \xi\nabla\mathrm{div}\,\boldsymbol{u}^0\right]\right), \end{aligned} \tag{3.48}$$

for all $\boldsymbol{\psi} \in X_m$.

Remark 3.4.6 (Sense of the initial conditions)**.** *Note that the term $\boldsymbol{F}(0)$ appearing in the definition of the initial condition $\boldsymbol{u}_t^m(0)$ in (3.48) has a sense because of the embedding $H^1(0,T;L^2(\Omega)^N) \subset \mathcal{C}([0,T];L^2(\Omega)^N)$.*

The following lemma gives additional estimates of $\boldsymbol{u}_t^m$.

Lemma 3.4.7. *Let $\boldsymbol{u}^0 \in H^2(\Omega)^N \cap H_0^1(\Omega)^N$ and $\boldsymbol{F} \in H^1(0,T;L^2(\Omega)^N)$. Then there exist an independent of m constant B_2 such that the approximations $\boldsymbol{u}^m$ satisfy the following estimates*

$$\left.\begin{aligned} &\|\boldsymbol{u}_t^m\|^2_{L^2(0,T;H_0^1(\Omega)^N)} \\ &\|\boldsymbol{u}_t^m\|^2_{L^\infty(0,T;L^2(\Omega)^N)} \end{aligned}\right\} \le B_2 \cdot \left[\left\|\boldsymbol{u}^0\right\|^2_{H^2(\Omega)^N} + \|\boldsymbol{F}(0)\|^2_{L^2(\Omega)^N} + T\,\|\boldsymbol{F}_t\|^2_{L^2(0,T;L^2(\Omega)^N)}\right].$$

Proof. Similar to the proof of Lemma 3.4.5, substitute $\boldsymbol{\psi} = \boldsymbol{u}_t^m$ into (3.48) and integrate over $(0,t)$, $t \le T$, to obtain

$$\begin{aligned} &\frac{\rho_0}{2}\int_\Omega |\boldsymbol{u}_t^m(t)|^2\,\mathrm{d}\boldsymbol{x} + \int_0^t\int_\Omega \left[\mu\,|\nabla\boldsymbol{u}_t^m|^2 + \xi|\mathrm{div}\,\boldsymbol{u}_t^m|^2\right]\mathrm{d}\boldsymbol{x}\,\mathrm{d}s \\ &\quad \le \frac{\rho_0}{2}\int_\Omega |\boldsymbol{u}_t^0|^2\,\mathrm{d}\boldsymbol{x} + \int_0^t\int_\Omega |\boldsymbol{F}_t(\tau)|\,|\boldsymbol{u}_t^m(s)|\ \mathrm{d}\boldsymbol{x}\,\mathrm{d}s. \end{aligned}$$

To apply the generalized Gronwall inequality (3.174), use Hölder's inequality to estimate the last integral over Ω as follows

$$\int_\Omega |\boldsymbol{F}_t(s)|\,|\boldsymbol{u}_t^m(s)| \le 2\left[\frac{1}{2\rho_0}\int_\Omega |\boldsymbol{F}_t(s)|^2\right]^{1/2}\cdot\left[\int_\Omega \frac{\rho_0}{2}\,|\boldsymbol{u}_t^m(s)|^2\right]^{1/2}.$$

Due to (3.174), we obtain

$$\frac{\rho_0}{2}\int_\Omega |\boldsymbol{u}_t^m(t)|^2\,\mathrm{d}\boldsymbol{x} + \int_0^t\int_\Omega \Big[\mu\,|\nabla \boldsymbol{u}_t^m|^2 + \xi\,|\mathrm{div}\,\boldsymbol{u}_t^m|^2\Big]\,\mathrm{d}\boldsymbol{x}\mathrm{d}s$$
$$\leq \rho_0 \int_\Omega |\boldsymbol{u}_t^0|^2\,\mathrm{d}\boldsymbol{x} + \frac{3t}{2\rho_0}\int_0^t\int_\Omega |\boldsymbol{F}_t(s)|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}s.$$

Note that $\boldsymbol{u}_t^0 \in L^2(\Omega)^N$ due to (3.48). □

3.4.1.3 Passage to the limit and additional regularity

The next lemma clarifies how solutions of problem (3.40) can be constructed from the considered approximations.

Lemma 3.4.8 (Passage to the limit)**.** *Let* $\boldsymbol{u}^0 \in H^2(\Omega)^N \cap H_0^1(\Omega)^N$ *and* $\boldsymbol{F} \in H^1(0,T;L^2(\Omega)^N)$ *for a given* $T > 0$. *Then there exists a unique function* $\boldsymbol{u}$ *that possesses the following regularity:*

$$\boldsymbol{u} \in L^2(0,T;H^2(\Omega)^N) \cap L^\infty(0,T;H_0^1(\Omega)^N),$$
$$\boldsymbol{u}_t \in L^\infty(0,T;L^2(\Omega)^N) \cap L^2(0,T;H_0^1(\Omega)^N)$$

and satisfies the following equations

$$\int_0^T\int_\Omega [\rho_0\,\boldsymbol{u}_t - \mu\Delta\boldsymbol{u} - \xi\nabla\mathrm{div}\,\boldsymbol{u} - \boldsymbol{F}]\cdot\boldsymbol{\phi}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = 0,$$

$$-\int_\Omega \boldsymbol{u}_t(0)\cdot\boldsymbol{\psi}(0)\,\mathrm{d}\boldsymbol{x} + \int_0^T\int_\Omega \Big[-\rho_0\boldsymbol{u}_t\cdot\boldsymbol{\psi}_t + \mu\,\nabla\boldsymbol{u}_t : \nabla\boldsymbol{\psi}$$
$$+\xi\,\mathrm{div}\,(\boldsymbol{u}_t)\,\mathrm{div}\,(\boldsymbol{\psi}) - \boldsymbol{F}_t\cdot\boldsymbol{\psi}\Big]\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = 0,$$

for all $\boldsymbol{\phi} \in L^2(0,T;L^2(\Omega)^N)$ *and all* $\boldsymbol{\psi} \in H^1(0,T;H_0^1(\Omega)^N)$, $\boldsymbol{\psi}(T) = \boldsymbol{0}$.

Proof. The estimates of the approximations $\boldsymbol{u}^m$ in Lemmas 3.4.5 and 3.4.7 are independent of m. Thus, there exist a function $\boldsymbol{u}$ and a subsequence again denoted by $\{\boldsymbol{u}^m\}$ that satisfies the following relations:

$$\begin{aligned} \boldsymbol{u}^m &\rightharpoonup \boldsymbol{u} && \text{weakly in } H^1(0,T;H_0^1(\Omega)^N),\\ \boldsymbol{u}^m &\rightharpoonup \boldsymbol{u} && \text{weakly in } L^2(0,T;H^2(\Omega)^N),\\ \boldsymbol{u}_t^m &\overset{*}{\rightharpoonup} \boldsymbol{u}_t && *\text{-weakly in } L^\infty(0,T;L^2(\Omega)^N). \end{aligned} \tag{3.49}$$

By construction of $\boldsymbol{u}^m$ (see (3.42)), it holds

$$\int_0^T\int_\Omega [\rho_0\,\boldsymbol{u}_t^m - \mu\Delta\boldsymbol{u}^m - \xi\nabla\mathrm{div}\,\boldsymbol{u}^m - \boldsymbol{F}]\cdot\boldsymbol{\psi} = 0, \quad \text{for all } \boldsymbol{\psi} \in L^2(0,T;X_m). \tag{3.50}$$

The convergence results (3.49) show that (3.50) remains true if $\boldsymbol{u}^m$ is replaced by the limit $\boldsymbol{u}$. Since

$$\bigcup_{m\in\mathbb{N}} L^2(0,T;X_m) \quad \text{is dense in} \quad L^2(0,T;L^2(\Omega)^N), \tag{3.51}$$

we obtain

$$\int_0^T \int_\Omega [\rho_0\, \boldsymbol{u}_t - \mu\Delta \boldsymbol{u} - \xi\nabla \mathrm{div}\, \boldsymbol{u} - \boldsymbol{F}] \cdot \boldsymbol{\psi} \;= 0 \qquad \text{for all } \boldsymbol{\psi} \in L^2(0,T; L^2(\Omega)^N). \tag{3.52}$$

This is the first equation claimed in the lemma.

To show the second one, note that $\boldsymbol{u}_t^m$ satisfies (3.48) and define

$$\boldsymbol{u}_t^0 := \rho_0^{-1} \left([\mu\Delta + \xi\nabla \mathrm{div}]\boldsymbol{u}^0 + \boldsymbol{F}(0) \right).$$

Due to (3.48), the approximation $\boldsymbol{u}_t^m$ satisfies the equation

$$- \int_\Omega P_{X_m}(\boldsymbol{u}_t^0) \cdot \boldsymbol{\psi}(0)\, \mathrm{d}\boldsymbol{x} + \int_0^T \int_\Omega \Big[- \rho_0\, \boldsymbol{u}_t^m \cdot \boldsymbol{\psi}_t + \mu\, \nabla \boldsymbol{u}_t^m : \nabla \boldsymbol{\psi} \\ + \xi\, \mathrm{div}\, (\boldsymbol{u}_t^m)\, \mathrm{div}\, (\boldsymbol{\psi}) - \boldsymbol{F}_t \cdot \boldsymbol{\psi} \Big]\, \mathrm{d}\boldsymbol{x}\mathrm{d}t = 0$$

for all $\boldsymbol{\psi} \in H^1(0,T; X_m)$, $\boldsymbol{\psi}(T) = \boldsymbol{0}$. Similar to (3.51), the set $\bigcup_{m\in\mathbb{N}} L^2(0,T; X_m)$ is dense in $L^2(0,T; H_0^1(\Omega)^N)$. Thus, the convergence result (3.49) yields:

$$- \int_\Omega \boldsymbol{u}_t^0 \cdot \boldsymbol{\psi}(0)\, \mathrm{d}\boldsymbol{x} + \int_0^T \int_\Omega \Big[- \rho_0 \boldsymbol{u}_t \cdot \boldsymbol{\psi}_t + \mu\, \nabla \boldsymbol{u}_t : \nabla \boldsymbol{\psi} \\ + \xi\, \mathrm{div}\, (\boldsymbol{u}_t)\, \mathrm{div}\, (\boldsymbol{\psi}) - \boldsymbol{F}_t \cdot \boldsymbol{\psi} \Big]\, \mathrm{d}\boldsymbol{x}\mathrm{d}t = 0 \tag{3.53}$$

for all $\boldsymbol{\psi} \in H^1(0,T; H_0^1(\Omega)^N)$, $\boldsymbol{\psi}(T) = \boldsymbol{0}$.

It remains to show that $\boldsymbol{u}_t(0) = \boldsymbol{u}_t^0$ holds. To this end, note that (3.53) implies that $\boldsymbol{u}_{tt}$ satisfies

$$\rho_0\, \boldsymbol{u}_{tt} = \boldsymbol{F}_t - [\mu\, \Delta + \xi\, \nabla \mathrm{div}]\, \boldsymbol{u}_t \qquad \in L^2(0,T; H^{-1}(\Omega)^N).$$

Moreover, $\boldsymbol{u}_t \in L^2(0,T; H_0^1(\Omega)^N)$ by the first relation of (3.49). Thus, Theorem 3.F.5 yields that $\boldsymbol{u}_t \in \mathcal{C}([0,T]; L^2(\Omega)^N)$. Choose the testfunction $\boldsymbol{\psi}$ in equation (3.53) in the following way. Fix an arbitrary $\boldsymbol{\eta} \in H_0^1(\Omega)^N$ and, for $\delta \in (0,T)$, define the function f_δ as follows:

$$f_\delta(t) = \begin{cases} 1 - t/\delta & \text{if } t \in [0,\delta], \\ 0 & \text{if } t > \delta. \end{cases}$$

Choose $\boldsymbol{\psi} = \boldsymbol{\psi}_\delta(\boldsymbol{x},t) := f_\delta(t)\, \boldsymbol{\eta}(\boldsymbol{x})$ in (3.53) and set $X := L^2(0,T; H_0^1(\Omega)^N)$. Then, Theorem 3.F.5 yields

$$\int_\Omega \left[\boldsymbol{u}_t(0) - \boldsymbol{u}_t^0 \right] \cdot \boldsymbol{\eta}\, \mathrm{d}\boldsymbol{x} = - \langle \rho_0\, \boldsymbol{u}_{tt}\;,\; \boldsymbol{\psi}_\delta \rangle_{X' \times X} \\ + \int_0^T \int_\Omega \Big[\boldsymbol{F}_t \cdot \boldsymbol{\psi}_\delta - \mu\, \nabla \boldsymbol{u}_t : \nabla \boldsymbol{\psi}_\delta - \xi\, \mathrm{div}\, (\boldsymbol{u}_t)\, \mathrm{div}\, (\boldsymbol{\psi}_\delta) \Big]\, \mathrm{d}\boldsymbol{x}\mathrm{d}t.$$

For $\delta \to 0$, we have $\boldsymbol{\psi}_\delta \to 0$ in X. Thus, the right-hand side of the above equation tends zero. The relation $\boldsymbol{u}_t(0) = \boldsymbol{u}_t^0$ follows because $\boldsymbol{\eta} \in H_0^1(\Omega)^N$ is arbitrary, and $H_0^1(\Omega)^N$ is dense in $L^2(\Omega)^N$.

The uniqueness of $\boldsymbol{u}$ follows from the linearity of equations (3.52) and (3.53). □

The next lemma establishes additional regularity of the function $\boldsymbol{u}$.

Lemma 3.4.9 (Additional regularity). *Assume the hypothesis of Lemma 3.4.8. Then, the function $\boldsymbol{u}$ lies in $L^\infty(0,T;H^2(\Omega)^N)$ and satisfies the estimate*

$$\|\boldsymbol{u}\|_{L^\infty(0,T;H^2(\Omega)^N)} \leq C \left[\|\boldsymbol{F}\|_{L^\infty(0,T;L^2(\Omega)^N)} + \|\boldsymbol{u}_t\|_{L^\infty(0,T;L^2(\Omega)^N)}\right].$$

Proof. By Lemma 3.4.8, we have

$$\int_0^T \int_\Omega [-\mu\Delta - \xi\nabla\mathrm{div}]\, \boldsymbol{u}\cdot\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \int_0^T \int_\Omega [\boldsymbol{F} - \rho_0\,\boldsymbol{u}_t]\cdot\boldsymbol{\psi}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \tag{3.54}$$

for all $\boldsymbol{\psi} \in L^2(0,T;L^2(\Omega)^N)$. The embedding $H^1(0,T;L^2(\Omega)^N) \subset \mathcal{C}([0,T],L^2(\Omega)^N)$ and Lemma 3.4.8 imply that $[\boldsymbol{F} - \rho_0\,\boldsymbol{u}_t] \in L^\infty(0,T;L^2(\Omega)^N)$. Since $L^2(0,T;L^2(\Omega)^N)$ is dense in $L^1(0,T;L^2(\Omega)^N)$, we obtain

$$[-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u} \in \left(L^1(0,T;L^2(\Omega)^N)\right)' = L^\infty(0,T;L^2(\Omega)^N).$$

The strong ellipticity of $[-\mu\Delta - \xi\nabla\mathrm{div}]$ and Theorem 3.G.2 yield that $\boldsymbol{u} \in L^\infty(0,T;H^2(\Omega)^N)$. The estimate claimed in the lemma follows from (3.54). □

Remark 3.4.10 (Scalar continuity). *Lemma 3.4.9 and Theorem 3.F.4 applied with $X = H^2(\Omega)^N$ and $Y = H^1_0(\Omega)^N$ yield $\boldsymbol{u} \in \mathcal{C}_s(0,T;H^2(\Omega)^N)$.*

3.4.1.4 Regularity of the right-hand side

In this section, we show that the function $\boldsymbol{F}$ defined by (3.39) satisfies $\boldsymbol{F} \in H^1(0,T;L^2(\Omega)^N)$ provided that $p^0 \in H^1(\Omega)$, $\boldsymbol{U}_b \in H^2(\Omega)^N$, and $\boldsymbol{w} \in W_0$ (see Definition 3.4.3). Further, we estimate the $H^1(0,T;L^2(\Omega)^N)$-norm of the difference $\boldsymbol{F}(\boldsymbol{w}_1) - \boldsymbol{F}(\boldsymbol{w}_2)$ for $\boldsymbol{w}_1$, $\boldsymbol{w}_2 \in W_0$.

Let us first estimate the pressure. By (3.38), the following inequalities hold for $t \in [0,T]$ and for C being sufficiently large:

$$\begin{aligned}
\int_0^t \int_\Omega |\nabla p_t|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau &= \frac{1}{\gamma^2}\int_0^t\int_\Omega |\nabla\mathrm{div}\,(\boldsymbol{U}_b + \boldsymbol{w})|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau, \\
&\leq C\,t\left[\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{L^\infty(0,T;H^2(\Omega)^N)}\right], \\
\int_\Omega |\nabla p(t)|^2\,\mathrm{d}\boldsymbol{x} &\leq C\left[\left\|p^0\right\|^2_{H^1(\Omega)} + t\left(\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{L^\infty(0,T;H^2(\Omega))}\right)\right], \\
\int_0^t\int_\Omega |\nabla p|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau &\leq C\,t\left[\left\|p^0\right\|^2_{H^1(\Omega)} + t\left(\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{L^\infty(0,T;H^2(\Omega))}\right)\right].
\end{aligned} \tag{3.55}$$

The next lemma gives estimates of the convective term.

Lemma 3.4.11 (The convective term)**.** *Let $\boldsymbol{V}$, $\boldsymbol{W} \in W$, and let $T > 0$ be finite. Then there exists a constant C_W such that*

$$\begin{aligned}
\|(\boldsymbol{W}\cdot\nabla)\boldsymbol{V}\|^2_{L^\infty(0,T;L^2(\Omega)^N)} &\le C_W\left[\|\boldsymbol{W}(0)\|^2_{H^1(\Omega)^N} + T\|\boldsymbol{W}\|^2_W\right] \\
&\quad\times\|\boldsymbol{V}\|_W\left[\|\boldsymbol{V}(0)\|^2_{H^1(\Omega)^N} + T\|\boldsymbol{V}\|^2_W\right]^{1/2}, \\
\|(\boldsymbol{W}\cdot\nabla)\boldsymbol{V}\|^2_{L^2(0,T;L^2(\Omega)^N)} &\le C_W\,T\|\boldsymbol{V}\|^2_W\cdot\|\boldsymbol{W}\|^2_W, \\
\left\|\frac{\partial}{\partial t}\,[(\boldsymbol{W}\cdot\nabla)\boldsymbol{V}]\right\|^2_{L^\infty(0,T;L^2(\Omega)^N)} &\le C_W\|\boldsymbol{V}\|^2_W\cdot\|\boldsymbol{W}\|^2_W.
\end{aligned}$$

The constant C_W is independent of $\boldsymbol{V}$, $\boldsymbol{W}$ and T.

Proof. Let v be an arbitrary component of $\boldsymbol{V}$, and w be an arbitrary component of $\boldsymbol{W}$. Then each component of $(\boldsymbol{W}\cdot\nabla)\boldsymbol{V}$ consists of a sum of terms having the form $v_{x_k}\cdot w$ where $k \in \{1,...,N\}$. Therefore, it is enough to estimate the product $v_{x_k}\cdot w$.

First, we establish some property of functions from $H^1(0,T;L^2(\Omega))$. Due to the generalized Minkowski inequality (see Theorem 3.A.4), a function $u \in H^1(0,T;L^2(\Omega))$ satisfies the following estimate

$$\begin{aligned}
\|u(t)\|^2_{L^2(\Omega)} &\le 2\int_\Omega |u(0)|^2\,\mathrm{d}\boldsymbol{x} + 2\int_\Omega\left[\int_0^t u_t(\tau)\,\mathrm{d}\tau\right]^2\mathrm{d}\boldsymbol{x} \\
&\le 2\int_\Omega |u(0)|^2\,\mathrm{d}\boldsymbol{x} + 2\left(\int_0^t\left[\int_\Omega |u_t(\tau)|^2\,\mathrm{d}\boldsymbol{x}\right]^{1/2}\mathrm{d}\tau\right)^2 \\
&\le 2\int_\Omega |u(0)|^2\,\mathrm{d}\boldsymbol{x} + 2t\int_0^t\int_\Omega |u_t|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau
\end{aligned}\tag{3.56}$$

for $t \in (0,T)$. Let us show the first inequality claimed in the lemma. Using Hölder's inequality, the auxiliary inequality (3.56) and the interpolation inequality (see Theorem 3.E.7) yield the following estimate:

$$\begin{aligned}
\int_\Omega |w(t)\,v_{x_k}(t)|^2 &\le \|w(t)\|^2_{L^6(\Omega)}\,\|v_{x_k}(t)\|^2_{L^3(\Omega)} \le C_\Omega\,\|w(t)\|^2_{H^1(\Omega)}\,\|v_{x_k}(t)\|^2_{H^{1/2}(\Omega)} \\
&\le C\left[\|w(0)\|^2_{H^1(\Omega)} + t\,\|w_t\|^2_{L^2(0,T;H^1(\Omega))}\right]\|v_{x_k}(t)\|_{H^1(\Omega)}\,\|v_{x_k}(t)\|_{L^2(\Omega)} \\
&\le C\left[\|w(0)\|^2_{H^1(\Omega)} + t\,\|w_t\|^2_{L^2(0,T;H^1(\Omega))}\right] \\
&\quad\times\|v_{x_k}(t)\|_{H^1(\Omega)}\left[\|v_{x_k}(0)\|^2_{L^2(\Omega)} + t\,\|v_{x_k,t}\|^2_{L^2(0,T;L^2(\Omega))}\right]^{1/2}.
\end{aligned}$$

This shows the validity of the first inequality claimed in the lemma. The second inequality follows from the first one and Hölder's inequality.

To obtain the third inequality, consider the time derivative

$$\frac{\partial(w\,v_{x_k})}{\partial t} = w_t\,v_{x_k} + w\,v_{x_k,t}. \tag{3.57}$$

The first term on the right-hand side of (3.57) can be estimated using the interpolation inequality and the embedding $H^1(\Omega) \subset L^6(\Omega)$ for $N \leq 3$. It holds

$$\begin{aligned}\int_0^t \int_\Omega |w_t\, v_{x_k}|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau &\leq \int_0^t \|w_t\|^2_{L^3(\Omega)} \cdot \|v_{x_k}\|^2_{L^6(\Omega)} \,\mathrm{d}\tau \\ &\leq C \int_0^t \|w_t\|_{H^1(\Omega)}\, \|w_t\|_{L^2(\Omega)}\, \|v_{x_k}\|^2_{H^1(\Omega)} \,\mathrm{d}\tau \\ &\leq C\, \|v\|^2_{L^\infty(0,T;H^2(\Omega))} \cdot \|w_t\|_{L^\infty(0,T;L^2(\Omega))} \cdot \|w_t\|_{L^1(0,T;H^1(\Omega))} \,.\end{aligned}$$

To estimate the second term in (3.57), use the embedding $H^2(\Omega) \subset \mathcal{C}(\overline{\Omega})$ for $N \leq 3$, and Hölder's inequality to obtain

$$\begin{aligned}\int_0^t \int_\Omega |w\, v_{x_k,t}|^2 \,\mathrm{d}\boldsymbol{x}\tau &\leq \int_0^t \max_{\boldsymbol{x}\in\bar{\Omega}} |w(\boldsymbol{x},\tau)|^2 \cdot \int_\Omega v_{x_k,t}(\tau)^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\tau \\ &\leq C_\Omega\, \|w\|^2_{L^\infty(0,T;H^2(\Omega))}\, \|v_t\|^2_{L^2(0,T;H^1(\Omega))} \,.\end{aligned}$$

This completes the proof of the third inequality claimed in the lemma. □

The next lemma shows that the function $\boldsymbol{F}$ defined in (3.39) lies in $H^1(0,T,L^2(\Omega)^N)$.

Lemma 3.4.12 (Regularity of $\boldsymbol{F}$). *Assume that* $\boldsymbol{u}^0 \in H^2(\Omega)^N \cap H^1_0(\Omega)^N$, $\boldsymbol{U}_b \in H^2(\Omega)^N$, $p^0 \in H^1(\Omega)$, *and* $\boldsymbol{f} \in H^1(0,T,L^2(\Omega)^N)$. *Further, let* $\boldsymbol{w} \in W_0$ *be given with* $\boldsymbol{w}(0) = \boldsymbol{u}^0$. *Set* $R_b := \|\boldsymbol{U}_b\|_{H^2(\Omega)^N} + \|\boldsymbol{w}\|_{W_0}$ *and define the function* g_F *as follows*

$$\begin{aligned}&g_F : [0,\infty)^2 \to [0,\infty), \\ &g_F(t,\, r) = R_b\big(\|\boldsymbol{U}_b\|_{H^1(\Omega)^N} + \big\|\boldsymbol{u}^0\big\|_{H^1_0(\Omega)^N}\big)^3 + T\, R_b^2 + T^{3/2}\, R_b^4.\end{aligned}$$

Then, there exist an independent of $\boldsymbol{w}$ *and* T *constant* B_F *such that the function* $\boldsymbol{F}$ *defined in* (3.39) *satisfies the following estimates*

$$\begin{aligned}\|\boldsymbol{F}\|^2_{L^2(0,T;L^2(\Omega)^N)} &\leq T\, B_F \cdot \big(1 + \|\boldsymbol{w}\|^2_{W_0} + \|\boldsymbol{w}\|^4_{W_0}\big), \\ \|\boldsymbol{F}_t\|^2_{L^2(0,T;L^2(\Omega)^N)} &\leq B_F \cdot \big(1 + \|\boldsymbol{w}\|^2_{W_0} + \|\boldsymbol{w}\|^4_{W_0}\big), \\ \|\boldsymbol{F}\|^2_{L^\infty(0,T;L^2(\Omega)^N)} &\leq B_F \cdot \big(1 + g_F(T,\, \|\boldsymbol{w}\|_{W_0})\big).\end{aligned}$$

Proof. Let us regard $\boldsymbol{U}_b$ as a constant in time function. Then it holds: $\|\boldsymbol{U}_b\|_W = \|\boldsymbol{U}_b\|_{H^2(\Omega)^N}$ (see Definition 3.4.3). To derive the first estimate of $\boldsymbol{F}$, use the definition (3.39), the estimate of the pressure (3.55), and Lemma 3.4.11. Applying Young's inequality several times yields

$$\begin{aligned}\int_0^T \int_\Omega |\boldsymbol{F}|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t \leq C\, T\Big[\, &\|\boldsymbol{f}\|^2_{L^\infty(0,T;L^2(\Omega)^N)} + \big\|p^0\big\|^2_{H^1(\Omega)} \\ &+ \|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{U}_b\|^4_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{W_0} + \|\boldsymbol{w}\|^4_{W_0}\Big].\end{aligned} \tag{3.58}$$

If B_F is chosen sufficiently large, the first estimate claimed in the lemma follows from (3.58). In the same way, the time derivative can be estimated as follows

$$\begin{aligned}\int_0^T \int_\Omega |\boldsymbol{F}_t|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t \leq C\Big[\, &\|\boldsymbol{f}_t\|^2_{L^2(0,T;L^2(\Omega)^N)} + \|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{U}_b\|^4_{H^2(\Omega)^N} \\ &+ \|\boldsymbol{w}\|^2_W + \|\boldsymbol{w}\|^4_W\Big].\end{aligned} \tag{3.59}$$

If B_F is sufficiently large, the second estimate claimed in the lemma follows from (3.59).

To obtain the third estimate, use (3.55) and Lemma 3.4.11 and proceed as follows

$$\begin{aligned}\int_\Omega |\boldsymbol{F}(t)|^2 \, \mathrm{d}\boldsymbol{x} \leq C \Big[&\|\boldsymbol{f}(t)\|^2_{L^2(\Omega)^N} \\ &+ \left\|p^0\right\|^2_{H^1(\Omega)} + t\big(\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{L^\infty(0,T;H^2(\Omega))}\big) \\ &+ \big(\|\boldsymbol{U}_b\|_{H^2(\Omega)^N} + \|\boldsymbol{w}\|_{W_0}\big) \\ &\times \Big(\|\boldsymbol{U}_b\|^2_{H^1(\Omega)^N} + \left\|\boldsymbol{u}^0\right\|^2_{H^1(\Omega)^N} + t\big[\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{W_0}\big]\Big)^{3/2}\Big].\end{aligned} \tag{3.60}$$

Due to the embedding $H^1(0,T;L^2(\Omega)^N) \subset \mathcal{C}([0,T];L^2(\Omega)^N)$, the first term on the right-hand side of (3.60) is bounded. To estimate the summands containing $\boldsymbol{w}$ on the right-hand side of (3.60), set $R_b = \|\boldsymbol{U}_b\|_{H^2(\Omega)^N} + \|\boldsymbol{w}\|_{W_0}$ and use the inequality $(a^2+b^2)^{1/2} \leq a + b$ that holds for $a,\, b > 0$. We have

$$\begin{aligned}&t\big(\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{L^\infty(0,T;H^2(\Omega))}\big) + \big(\|\boldsymbol{U}_b\|_{H^2(\Omega)^N} + \|\boldsymbol{w}\|_{W_0}\big) \\ &\quad\times \Big(\|\boldsymbol{U}_b\|^2_{H^1(\Omega)^N} + \left\|\boldsymbol{u}^0\right\|^2_{H^1(\Omega)^N} + t\big[\|\boldsymbol{U}_b\|^2_{H^2(\Omega)^N} + \|\boldsymbol{w}\|^2_{W_0}\big]\Big)^{3/2} \\ &\leq t\, R_b^2 + C\, R_b\big(\|\boldsymbol{U}_b\|_{H^1(\Omega)^N} + \left\|\boldsymbol{u}^0\right\|_{H^1_0(\Omega)^N}\big)^3 + t^{3/2}\, R_b^4.\end{aligned} \tag{3.61}$$

Substituting (3.61) into (3.60) and choosing sufficiently large B_F completes the proof of the third inequality claimed in the lemma. □

The next lemma gives estimates of the difference $\tilde{\boldsymbol{F}} := \boldsymbol{F}(\boldsymbol{w}_1) - \boldsymbol{F}(\boldsymbol{w}_2)$ for two given functions $\boldsymbol{w}_1,\, \boldsymbol{w}_2 \in W_0$.

Lemma 3.4.13 (Estimation of $\tilde{\boldsymbol{F}}$)**.** *Assume the hypothesis of Lemma 3.4.12. Let $\boldsymbol{w}_1,\, \boldsymbol{w}_2 \in W_0$ be given with $\boldsymbol{w}_i(0) = \boldsymbol{u}^0$, $i = 1, 2$, and let $\boldsymbol{F}(\boldsymbol{w}_1)$ and $\boldsymbol{F}(\boldsymbol{w}_2)$ be defined by* (3.39)*. Set $\tilde{\boldsymbol{w}} = \boldsymbol{w}_1 - \boldsymbol{w}_2$, $\tilde{\boldsymbol{F}} = \boldsymbol{F}(\boldsymbol{w}_1) - \boldsymbol{F}(\boldsymbol{w}_2)$, and $r = \max\{\|\boldsymbol{w}_j\|_{W_0} \,:\, j = 1, 2\}$. Then, there exists an independent of $\tilde{\boldsymbol{w}}$ and T constant $\tilde{B}_F$ such that $\tilde{\boldsymbol{F}}$ satisfies the following estimates*

$$\begin{aligned}\left\|\tilde{\boldsymbol{F}}\right\|_{L^2(0,T;L^2(\Omega)^N)} &\leq T^{1/2}\, \tilde{B}_F\, \|\tilde{\boldsymbol{w}}\|_{W_0}, \\ \left\|\tilde{\boldsymbol{F}}_t\right\|_{L^2(0,T;L^2(\Omega)^N)} &\leq \tilde{B}_F\, \|\tilde{\boldsymbol{w}}\|_{W_0}, \\ \left\|\tilde{\boldsymbol{F}}\right\|_{L^\infty(0,T;L^2(\Omega)^N)} &\leq \tilde{B}_F \left[T^{1/2} + T^{3/4}\right] \|\tilde{\boldsymbol{w}}\|_{W_0}.\end{aligned}$$

The constant $\tilde{B}_F$ is nondecreasing in r.

Proof. Set $\boldsymbol{W}_i = \boldsymbol{U}_b + \boldsymbol{w}_i$ for $i = 1, 2$. Then, $\tilde{\boldsymbol{F}}$ is given by the formula (see (3.39)):

$$\tilde{\boldsymbol{F}} = \nabla\tilde{p} - \rho_0\left[(\boldsymbol{W}_1 \cdot \nabla)\tilde{\boldsymbol{w}} + (\tilde{\boldsymbol{w}} \cdot \nabla)\boldsymbol{W}_2\right]. \tag{3.62}$$

where the difference $\tilde{p} = p_1 - p_2$ is determined by the relations

$$\tilde{p}_t = -\frac{1}{\gamma}\,\mathrm{div}\,\tilde{\boldsymbol{w}}, \qquad \tilde{p} = -\frac{1}{\gamma}\int_0^t \mathrm{div}\,\tilde{\boldsymbol{w}}(\tau)\,\mathrm{d}\tau. \tag{3.63}$$

Using formula (3.62), the generalized Minkowski inequality (see Theorem 3.A.4), and Lemma 3.4.11 yields

$$\int_0^T \int_\Omega |\tilde{\boldsymbol{F}}|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t \le C\,T\left[\|\tilde{\boldsymbol{w}}\|_{W_0}^2 + \left(\|\boldsymbol{W}_1\|_W^2 + \|\boldsymbol{W}_2\|_W^2\right) \cdot \|\tilde{\boldsymbol{w}}\|_{W_0}^2\right]. \tag{3.64}$$

Similarly, the time derivative $\boldsymbol{F}_t$ can be estimated as follows

$$\int_0^T \int_\Omega |\tilde{\boldsymbol{F}}_t|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t \le C\left[\|\tilde{\boldsymbol{w}}\|_{W_0}^2 + \left(\|\boldsymbol{W}_1\|_W^2 + \|\boldsymbol{W}_2\|_W^2\right) \cdot \|\tilde{\boldsymbol{w}}\|_{W_0}^2\right]. \tag{3.65}$$

Note that $\|\boldsymbol{W}_i\|_W^2 \le 2\|\boldsymbol{U}_b\|_W^2 + 2\|\boldsymbol{w}_i\|_{W_0}^2$, $i = 1, 2$, and set $r = \max\{\|\boldsymbol{w}_1\|_{W_0}, \|\boldsymbol{w}_2\|_{W_0}\}$. The first and second inequalities claimed in the lemma follow from (3.64) and (3.65), if $\tilde{B}_F$ is chosen sufficiently large.

To obtain the estimate in $L^\infty(0,T;L^2(\Omega)^N)$, estimate the summands on the right-hand side of (3.62). Due to (3.63) and Theorem 3.A.4, it holds

$$\|\nabla\tilde{p}(t)\|_{L^2(\Omega)^N}^2 \le \frac{t}{\gamma^2}\,\|\tilde{\boldsymbol{w}}\|_{L^\infty(0,T;H^2(\Omega))}^2. \tag{3.66}$$

To estimate the nonlinear term on the right-hand side of (3.62), note that $\boldsymbol{w}_1(0) = \boldsymbol{w}_2(0)$ by the hypothesis of the lemma and use Lemma 3.4.11 to obtain:

$$\int_\Omega \left[(\boldsymbol{W}_1(t)\cdot\nabla)\tilde{\boldsymbol{w}}(t) + (\tilde{\boldsymbol{w}}(t)\cdot\nabla)\boldsymbol{W}_2(t)\right]^2 \le C\,t^{3/2}\left[\|\boldsymbol{U}_b\|_{H^2(\Omega)^N} + r\right]^2 \cdot \|\tilde{\boldsymbol{w}}\|_{W_0}^2. \tag{3.67}$$

To show the third inequality claimed in the lemma, combine (3.62), (3.66), and (3.67) and enlarge B_F if necessary. □

3.4.1.5 Fixed-point method

The goal of this section is to complete the proof of Theorem 3.4.4. The Lemmas 3.4.8, 3.4.9, and 3.4.12 show that $\boldsymbol{w} \in W_0$ implies $\boldsymbol{u} \in W_0$, where $\boldsymbol{u}$ is the solution of problem (3.40). Thus, the following definition makes sense.

Definition 3.4.14. *Assume that* $\boldsymbol{u}^0 \in H^2(\Omega)^N \cap H_0^1(\Omega)^N$, $\boldsymbol{U}_b \in H^2(\Omega)^N$, $p^0 \in H^1(\Omega)$, *and* $\boldsymbol{f} \in H^1(0,T;L^2(\Omega)^N)$. *The solution-operator G is defined as follows:*

$$G : W_0 \longrightarrow W_0, \quad G(\boldsymbol{w}) := \boldsymbol{u},$$

where $\boldsymbol{u}$ *is the solution of the initial-boundary value problem* (3.40).

We proceed as follows.

- Estimate the norm of $G(\boldsymbol{w})$ in terms of $\boldsymbol{w}$ and T (Lemma 3.4.15).
- Estimate the norm of $G(\boldsymbol{w}_1) - G(\boldsymbol{w}_2)$ in terms of $\boldsymbol{w}_1 - \boldsymbol{w}_2$ and T (Lemma 3.4.16).
- Use Banach's fixed-point theorem to show that Theorem 3.4.4 holds true for sufficiently small T (Lemma 3.4.17).

Lemma 3.4.15. *Assume $\boldsymbol{w} \in W_0$ with $\boldsymbol{w}(0) = \boldsymbol{u}^0$ and denote $\boldsymbol{u} = G(\boldsymbol{w})$, where G is the mapping of defined by 3.4.14. Define a function g_u as follows:*

$$g_u : [0,\infty)^2 \to [0,\infty), \quad g_u(t,\, r) = r + r^2 + t^{1/4}\, r^2.$$

Then, there exists an independent of $\boldsymbol{w}$ constant B_G such that the following estimate holds true:

$$\|\boldsymbol{u}\|_{W_0} \leq B_G \left(1 + \|\boldsymbol{w}\|_{W_0}^{1/2} + T^{1/2}\, g_u(T, \|\boldsymbol{w}\|_{W_0})\right).$$

The constant B_G is nondecreasing in T.

Proof. Due to Lemmas 3.4.5 and 3.4.7, the following estimate holds

$$\left.\begin{array}{l} \|\boldsymbol{u}\|_{L^\infty(0,T;H_0^1(\Omega)^N)} \\ \|\boldsymbol{u}\|_{L^2(0,T;H^2(\Omega)^N)} \\ \|\boldsymbol{u}_t\|_{L^\infty(0,T;L^2(\Omega)^N)} \\ \|\boldsymbol{u}_t\|_{L^2(0,T;H_0^1(\Omega)^N)} \end{array}\right\} \leq C \left\{ \begin{array}{l} \left\|\boldsymbol{u}^0\right\|_{H^2(\Omega)^N} + \|\boldsymbol{F}(0)\|_{L^2(\Omega)^N} \\ + \|\boldsymbol{F}\|_{L^2(0,T;L^2(\Omega)^N)} + T^{1/2} \|\boldsymbol{F}_t\|_{L^2(0,T;L^2(\Omega)^N)} \end{array} \right\}. \tag{3.68}$$

Due to the definition of $\boldsymbol{F}$ (see (3.39)), the second term on the right-hand side can be estimated as follows

$$\|\boldsymbol{F}(0)\|_{L^2(\Omega)^N} \leq C \left[\|\boldsymbol{f}(0)\|_{L^2(\Omega)^N} + \left\|p^0\right\|_{H^1(\Omega)} + \|\boldsymbol{U}_b\|_{H^2(\Omega)^N}^2 + \left\|\boldsymbol{u}^0\right\|_{H^2(\Omega)^N}^2 \right]. \tag{3.69}$$

The third and fourth terms on the right-hand side of (3.68) can be estimated using Lemma 3.4.12 as follows

$$\|\boldsymbol{F}\|_{L^2(0,T;L^2(\Omega)^N)} + T^{1/2}\ \|\boldsymbol{F}_t\|_{L^2(0,T;L^2(\Omega)^N)} \leq C\, T^{1/2} \left(1 + \|\boldsymbol{w}\|_{W_0} + \|\boldsymbol{w}\|_{W_0}^2\right). \tag{3.70}$$

Substituting (3.69) and (3.70) into (3.68) yields

$$\left.\begin{array}{l} \|\boldsymbol{u}\|_{L^\infty(0,T;H_0^1(\Omega)^N)} \\ \|\boldsymbol{u}\|_{L^2(0,T;H^2(\Omega)^N)} \\ \|\boldsymbol{u}_t\|_{L^\infty(0,T;L^2(\Omega)^N)} \\ \|\boldsymbol{u}_t\|_{L^2(0,T;H_0^1(\Omega)^N)} \end{array}\right\} \leq C_2(T) + T^{1/2} C_1 \left(\|\boldsymbol{w}\|_{W_0} + \|\boldsymbol{w}\|_{W_0}^2\right), \tag{3.71}$$

where C_1 is independent of $\boldsymbol{w}$ and T, and C_2 is independent of $\boldsymbol{w}$.

It remains to estimate $\boldsymbol{u}$ in $L^\infty(0,T;H^2(\Omega)^N)$ (see the Definition 3.4.3). By Lemmas 3.4.9 and 3.4.12, and estimate (3.71), it holds

$$\begin{aligned} \|\boldsymbol{u}\|_{L^\infty(0,T;H^2(\Omega)^N)} &\leq \|\boldsymbol{F}\|_{L^\infty(0,T;L^2(\Omega)^N)} + \|\boldsymbol{u}_t\|_{L^\infty(0,T;L^2(\Omega)^N)} \\ &\leq B_F^{1/2}\, g_F(T, \|\boldsymbol{w}\|_{W_0})^{1/2} + C_2(T) + T^{1/2} C_1 \left(\|\boldsymbol{w}\|_{W_0} + \|\boldsymbol{w}\|_{W_0}^2\right), \end{aligned} \tag{3.72}$$

where g_F is the function defined in Lemma 3.4.12. The term $\sqrt{g_F(T, \|\boldsymbol{w}\|_{W_0})}$ can be estimated using Young's inequality and the inequality $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ that is true for $a,\, b \geq 0$. We have

$$\sqrt{g_F(T, \|\boldsymbol{w}\|_{W_0})} \leq C_3(T) + C_4\, \|\boldsymbol{w}\|_{W_0}^{1/2} + T^{1/2}\, \|\boldsymbol{w}\|_{W_0} + T^{3/4}\, \|\boldsymbol{w}\|_{W_0}^2. \tag{3.73}$$

Substituting (3.73) into (3.72) and combining (3.71) with (3.72) completes the proof. □

Lemma 3.4.16. *Let G be the mapping introduced by Definition 3.4.14. Let $\boldsymbol{w}_i \in W_0$ be given, and $\boldsymbol{w}_i(0) = \boldsymbol{u}^0$, $i = 1, 2$. Set $\boldsymbol{u}_i := G(\boldsymbol{w}_i)$, $\tilde{\boldsymbol{u}} := \boldsymbol{u}_1 - \boldsymbol{u}_2$, and $\tilde{\boldsymbol{w}} := \boldsymbol{w}_1 - \boldsymbol{w}_2$. Then, there exists an independent of $\tilde{\boldsymbol{w}}$ and T constant B_u such that $\tilde{\boldsymbol{u}}$ satisfies the following estimate*

$$\|\tilde{\boldsymbol{u}}\|_{W_0} \leq \tilde{B}_u \left[T^{1/2} + T^{3/4}\right] \|\tilde{\boldsymbol{w}}\|_{W_0}.$$

The constant $\tilde{B}_u$ is nondecreasing in r, where $r = \max\{\|\boldsymbol{w}_1\|_{W_0}, \|\boldsymbol{w}_2\|_{W_0}\}$.

Proof. The function $\tilde{\boldsymbol{u}}$ is a weak solution of the following initial boundary value problem (see (3.40)):

$$\begin{aligned} \rho_0 \tilde{\boldsymbol{u}}_t - \mu \Delta \tilde{\boldsymbol{u}} - \xi \nabla \operatorname{div} \tilde{\boldsymbol{u}} = \tilde{\boldsymbol{F}} \quad & \text{in } \Omega \times (0,T), \\ \tilde{\boldsymbol{u}} = \boldsymbol{0} \quad & \text{in } \partial\Omega \times (0,T), \\ \tilde{\boldsymbol{u}}(\boldsymbol{x}, 0) = \boldsymbol{0} \quad & \text{in } \Omega \times \{t = 0\}, \end{aligned}$$

where the right-hand side $\tilde{\boldsymbol{F}}$ is defined in (3.62). This problem is similar to (3.40). Therefore, $\tilde{\boldsymbol{u}}$ satisfies the estimate (3.68), if $\boldsymbol{u}^0$ and $\boldsymbol{F}$ are replaced by $\tilde{\boldsymbol{u}}^0$ and $\tilde{\boldsymbol{F}}$, respectively. Note that $\tilde{\boldsymbol{F}}(0) = \tilde{\boldsymbol{u}}^0 = \boldsymbol{0}$. Thus, it holds

$$\left.\begin{array}{l} \|\tilde{\boldsymbol{u}}\|_{L^\infty(0,T;H_0^1(\Omega)^N)} \\ \|\tilde{\boldsymbol{u}}\|_{L^2(0,T;H^2(\Omega)^N)} \\ \|\tilde{\boldsymbol{u}}_t\|_{L^\infty(0,T;L^2(\Omega)^N)} \\ \|\boldsymbol{u}_t\|_{L^2(0,T;H_0^1(\Omega)^N)} \end{array}\right\} \leq C \left\{ \left\|\tilde{\boldsymbol{F}}\right\|_{L^2(0,T;L^2(\Omega)^N)} + T^{1/2} \left\|\tilde{\boldsymbol{F}}_t\right\|_{L^2(0,T;L^2(\Omega)^N)} \right\}.$$

Apply Lemma 3.4.13 to obtain

$$\left.\begin{array}{l} \|\tilde{\boldsymbol{u}}\|_{L^\infty(0,T;H_0^1(\Omega)^N)} \\ \|\tilde{\boldsymbol{u}}\|_{L^2(0,T;H^2(\Omega)^N)} \\ \|\tilde{\boldsymbol{u}}_t\|_{L^\infty(0,T;L^2(\Omega)^N)} \\ \|\boldsymbol{u}_t\|_{L^2(0,T;H_0^1(\Omega)^N)} \end{array}\right\} \leq C\, T^{1/2}\, \tilde{B}_F \, \|\tilde{\boldsymbol{w}}\|_{W_0}. \tag{3.74}$$

It remains to estimate the $L^\infty(0,T;H^2(\Omega)^N)$-norm of $\tilde{\boldsymbol{u}}$. Similar to (3.72), $\tilde{\boldsymbol{u}}$ satisfies the following estimate

$$\|\tilde{\boldsymbol{u}}\|_{L^\infty(0,T;H^2(\Omega)^N)} \leq \left\|\tilde{\boldsymbol{F}}\right\|_{L^\infty(0,T;L^2(\Omega)^N)} + \|\tilde{\boldsymbol{u}}_t\|_{L^\infty(0,T;L^2(\Omega)^N)}. \tag{3.75}$$

The first term on the right-hand side of (3.75) is already estimated in the last inequality of Lemma 3.4.13. Combining the estimates (3.74) and (3.75) and applying Lemma 3.4.13 yield

$$\|\tilde{\boldsymbol{u}}\|_{W_0} \leq C\, \tilde{B}_F \left[T^{1/2} + T^{3/4}\right] \|\tilde{\boldsymbol{w}}\|_{W_0}.$$

Remember that $\tilde{B}_F$ is nondecreasing in r, where $r = \max\{\|\boldsymbol{w}_1\|_{W_0}, \|\boldsymbol{w}_2\|_{W_0}\}$. □

Lemma 3.4.17 (Fixed-point of G)**.** *Let B_G be the same constant as in Lemma 3.4.15. For $T > 0$ and $r > \left\|\boldsymbol{u}^0\right\|_{H^2(\Omega)^N}$, define the set*

$$M(T, r) := \left\{\boldsymbol{w} \in W_0(0,T) \;:\; \|\boldsymbol{w}\|_{W_0} \leq r \;\; and \;\; \boldsymbol{w}(0) = \boldsymbol{u}^0\right\}.$$

Then, for sufficiently large r, there exists $T_* \in (0, T]$ such that the solution operator G defined in 3.4.14 has a unique fixed-point $\boldsymbol{w}_* \in M(T_*, r)$.

Proof. The lemma follows from Banach's fixed-point theorem. To apply this theorem, we determine r and T_* such that $G(M(T_*, r)) \subset M(T_*, r)$. Let $T > 0$ be given. Due to Lemma 3.4.15, the following estimates hold

$$\begin{aligned} \|\boldsymbol{u}\|_{W_0(0,T_*)} &\leq B_G \left(1 + \|\boldsymbol{w}\|_{W_0}^{1/2} + T_*^{1/2}\, g_u(T, \|\boldsymbol{w}\|_{W_0(0,T_*)})\right) \\ &\leq B_G \left(1 + r^{1/2} + T_*^{1/2}\, g_u(T, r)\right) \end{aligned} \tag{3.76}$$

for $T_* \in (0, T]$, $r > \left\|\boldsymbol{u}^0\right\|_{H^2(\Omega)^N}$, and $\boldsymbol{w} \in M(T_*, r)$. In order to ensure the inclusion $G(M(T_*, r)) \subset M(T_*, r)$, we determine T_* and r such that $B_G \left(1 + r^{1/2} + T_*^{1/2}\, g_u(T, r)\right) \leq r$. To this end, note that the inequality

$$B_G(1 + r^{1/2}) < r \tag{3.77}$$

holds if, for example, $r > (3B_G^2)/2 + B_G$. Thus, if r satisfies (3.77), the estimates (3.76) imply the relation $G(M(T_*, r)) \subset M(T_*, r)$, if T_* satisfies the inequality

$$T_* \leq T_{\max} := \left[\frac{r - B_G(1 - \sqrt{r})}{B_G\, g_u(T, r)}\right]^2. \tag{3.78}$$

The next step is to show that G is contractive on $M(T_*, r)$ for sufficiently small T_*. Fix $r > 0$ satisfying (3.77). Then, the constant $\tilde{B}_u = \tilde{B}_u(r)$ of Lemma 3.4.16 is fixed. For two functions $\boldsymbol{w}_1$, $\boldsymbol{w}_2 \in M(T_*, r)$, denote $\boldsymbol{u}_i = G(\boldsymbol{w}_i)$, $i = 1, 2$, $\tilde{\boldsymbol{w}} = \boldsymbol{w}_1 - \boldsymbol{w}_2$, and $\tilde{\boldsymbol{u}} = \boldsymbol{u}_1 - \boldsymbol{u}_2$. By Lemma 3.4.16, the following estimate holds

$$\|\tilde{\boldsymbol{u}}\|_{W_0(0,T_*)} \leq \tilde{B}_u\, T_*^{1/2} \left[1 + T_{\max}^{1/4}\right] \|\tilde{\boldsymbol{w}}\|_{W_0(0,T_*)} \tag{3.79}$$

for any $T_* \in (0, T_{\max}]$. Choose $\delta \in (0, 1)$. Then, estimate (3.79) yields that $\|\tilde{\boldsymbol{u}}\|_{W_0} \leq \delta \|\tilde{\boldsymbol{w}}\|_{W_0}$, if T_* additionally satisfies the inequality

$$T_* \leq \left[\frac{\delta}{\tilde{B}_u\, [1 + T_{\max}]}\right]^2. \tag{3.80}$$

Thus, if r satisfies inequality (3.77) and T_* satisfies the inequalities (3.78) and (3.80), then we have $G(M(T_*, r)) \subset M(T_*, r)$ and $\|\tilde{\boldsymbol{u}}\|_{W_0} \leq \delta\, \|\tilde{\boldsymbol{w}}\|_{W_0}$. Due to Banach's fixed-point theorem, the solution-operator G has a unique fixed-point $\boldsymbol{w}_* \in M(T_*, r)$. □

To complete the proof of Theorem 3.4.4, use the second forumla of (3.38) to compute the pressure p. Then, the pair of functions $(\boldsymbol{w}_*, p)$ is a unique weak solution of (3.37) on the time interval $(0, T_*)$. Theorem 3.4.4 is proved.

This completes the investigation of the flow problem. The next section deals with the evolution of the particle density.

3.4.2 Evolution of the particle density

This section is devoted to the theoretical investigation of the initial boundary value problem (2.5) describing the evolution of the particle density. Here, we assume that the initial surface mass density η^0 on the active part Γ is given by the relation $\eta^0 = H(\rho^0)$, where the function H is defined in (2.67). The initial particle density ρ^0 is assumed to be nonnegative. Thus, the following initial boundary value problem is considered:

$$\begin{aligned}
\rho_t + \boldsymbol{U}\cdot\nabla\rho - \Delta\rho &= 0 && \text{in } \Omega\times(0,T),\\
-\partial_{\boldsymbol{\nu}}\rho &= 0 && \text{on } \big(\partial\Omega\setminus\big[\Gamma\cup\Gamma^{\text{in}}\big]\big)\times(0,T),\\
-\partial_{\boldsymbol{\nu}}\rho &= (\rho-g)\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| && \text{on } \Gamma^{\text{in}}\times(0,T),\\
\eta_t = -\partial_{\boldsymbol{\nu}}\rho, \quad \eta &= \mathcal{A}(\rho) && \text{on } \Gamma\times(0,T),\\
\rho(\boldsymbol{x},0) &= \rho^0(\boldsymbol{x}) \geq 0 && \text{on } \Omega\times\{t=0\},\\
\eta(\boldsymbol{x},0) = \eta^0(\boldsymbol{x}) &= H(\rho^0(\boldsymbol{x})) \geq 0 && \text{on } \Gamma\times\{t=0\},
\end{aligned} \tag{3.81}$$

where the operator $\mathcal{A}$ is defined as follows (see (2.67)):

$$\mathcal{A}(\rho(\boldsymbol{x},\cdot))(t) = \operatorname*{ess\,sup}_{0\leq s\leq t} H(\rho(\boldsymbol{x},s)). \tag{3.82}$$

Remark 3.4.18. *Note that, if the requirement $\eta^0 = H(\rho^0)$ is omitted, then the initial condition for η has to be replaced by the following relation*

$$\eta(\boldsymbol{x},0) = \max\left\{\eta^0(\boldsymbol{x})\,,\ H(\rho^0(\boldsymbol{x}))\right\} \quad \text{on } \Gamma\times\{t=0\}.$$

In this case the operator $\mathcal{A}$ is given as follows

$$\mathcal{A}(\rho(\boldsymbol{x},\cdot))(t) = \max\left\{\eta(\boldsymbol{x},0)\,,\ \operatorname*{ess\,sup}_{0\leq s\leq t} H(\rho(\boldsymbol{x},s))\right\}$$

instead of (3.82).

In this section, we suppose that the velocity field $\boldsymbol{U}(\boldsymbol{x},t)$ is a known function having the following properties

$$\begin{aligned}
&\boldsymbol{U}_b\cdot\boldsymbol{\nu} \leq 0 && \text{on } \Gamma^{\text{in}},\\
&\boldsymbol{U}_b\cdot\boldsymbol{\nu} \geq 0 && \text{on } \Gamma^{\text{out}},\\
&\boldsymbol{U}_b = \boldsymbol{0} && \text{on } \partial\Omega\setminus\big[\Gamma^{\text{in}}\cup\Gamma^{\text{out}}\big],\\
&\boldsymbol{U}\in\mathcal{C}([0,T];H^{3/2+\epsilon}(\Omega)^N)
\end{aligned} \tag{3.83}$$

for some $\epsilon > 0$. In (3.83), the trace $\boldsymbol{U}_b = \boldsymbol{U}|_{\partial\Omega}$ of the velocity field is assumed to be constant in time. Note that the last requirement in (3.83) and the embedding $H^s(\Omega)\subset\mathcal{C}(\overline{\Omega})$, $s > N/2$, yield the estimate

$$|\boldsymbol{U}(\boldsymbol{x},t)| \leq C_U, \qquad \text{for } t\in[0,T],\ \boldsymbol{x}\in\overline{\Omega}$$

for a suitable constant C_U.

In order to obtain the uniqueness of solutions in Section 3.4.2.5, the following additional regularity of the velocity field $\boldsymbol{U}$ is necessary: The norm $\|\operatorname{div} \boldsymbol{U}(t)\|_{L^\infty(\Omega)}$ (considered as function of t) is supposed to lie in the space $L^\infty(0,T)$. In this case, there exists a constant C_U^* such that

$$\|\operatorname{div} \boldsymbol{U}(t)\|_{L^\infty(\Omega)} \le C_U^* \qquad \text{for almost all } t \in (0,T). \tag{3.84}$$

To define weak solutions of problem (3.81), denote the trace on Γ of a function u defined in Ω by $\gamma_0\, u$. Weak solutions of (3.81) are defined as follows.

Definition 3.4.19 (Weak solutions)**.** *A pair of functions $(\rho,\, \eta)$,*

$$\begin{aligned} &\rho \in H^1(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)),\\ &\eta \in H^1(0,T;L^2(\Gamma)), \end{aligned}$$

is called weak solution of problem (3.81)*, if they satisfy the initial conditions, the relation*

$$\eta(\boldsymbol{x},t) = \mathcal{A}(\gamma_0\, \rho(\boldsymbol{x},\cdot))(t) \quad \textit{for almost all } (\boldsymbol{x},t) \in \Gamma \times (0,T), \tag{3.85}$$

and the following integral identity

$$\begin{aligned} &\int_0^T \int_\Omega [\rho_t + \boldsymbol{U}\cdot\nabla\rho]\,\psi\,\mathrm{d}\boldsymbol{x}\mathrm{d}t + \int_0^T\int_\Omega \nabla\rho\cdot\nabla\psi\,\mathrm{d}\boldsymbol{x}\mathrm{d}t\\ &\quad+\int_0^T\int_\Gamma \eta_t\,\psi\,\mathrm{d}s\mathrm{d}t + \int_0^T\int_{\Gamma^{\mathrm{in}}} \rho\,\psi|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\mathrm{d}t = \int_0^T\int_{\Gamma^{\mathrm{in}}} g\,\psi|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\mathrm{d}t, \end{aligned} \tag{3.86}$$

which holds for all testfunctions $\psi \in L^2(0,T;H^1(\Omega))$.

Remark 3.4.20. *It should be noted here that the relation* (3.85) *requires more regularity from the function ρ to define correctly the operator $\mathcal{A}(\gamma_0\,\rho)$. We will show in Section 3.4.2.4 that ρ is continuous in the variables $(z,\, t)$ for almost all (x,y), which eliminates all problems concerning the treatment of $\mathcal{A}(\gamma_0\rho)$.*

The main result of the present section is formulated in the following theorem.

Theorem 3.4.21 (Main result for the evolution of the particle density)**.** *Let $\Omega \in \mathbb{R}^N$ be a bounded Lipschitz domain. Assume $\rho^0 \in H^1(\Omega)\cap L^\infty(\Omega)$, $\rho^0 \ge 0$, $\eta^0 = H(\rho^0)$ in Γ, $g \in L^\infty(\Gamma^{\mathrm{in}})$ is constant in time, and $\boldsymbol{U}$ satisfies* (3.83)*.*

Then, for every $T>0$, there exists a weak solution $(\rho,\, \eta)$ to problem (3.81) *such that*

$$\begin{aligned} &\rho \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^{(3-\epsilon')/2}(\Omega)) \cap L^\infty(\Omega\times(0,T)),\\ &\eta \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{1/2}(\Gamma)), \end{aligned}$$

for any $\epsilon' > 0$. The function ρ satisfies the estimates:

$$0 \le \rho(\boldsymbol{x},t) \le \max\left\{\left\|\rho^0\right\|_{L^\infty(\Omega)},\, \|g\|_{L^\infty(\Gamma^{\mathrm{in}})}\right\} \quad \textit{a.e. in } \Omega\times(0,T).$$

If the velocity field $\boldsymbol{U}$ additionally satisfies estimate (3.84)*, then $(\rho,\, \eta)$ is a unique weak solution of problem* (3.81)*.*

3.4.2.1 Construction of approximate solutions

In this section, we construct approximate solutions to problem (3.81). To this end, construct an implicit time discretization scheme as follows. Fix an arbitrary $K \in \mathbb{N}$ and set $\tau = T/K$. Define functions ρ^n, $n \in \{1, 2, \ldots, K\}$ as solutions of the following problem:

$$\begin{aligned} \rho^n - \rho^{n-1} &= \tau \left[\Delta\rho^n + \boldsymbol{U} \cdot \nabla\rho^n\right] && \text{in } \Omega, \\ \eta^n - \eta^{n-1} &= -\tau\, \partial_{\boldsymbol{\nu}} \rho^n && \text{on } \Gamma, \\ -\partial_{\boldsymbol{\nu}}\, \rho^n &= (g - \rho^n)\, \boldsymbol{U}_b \cdot \boldsymbol{\nu} && \text{on } \Gamma^{\text{in}}, \\ \partial_{\boldsymbol{\nu}} \rho^n &= \boldsymbol{0} && \text{on } \partial\Omega \setminus \left[\Gamma \cup \Gamma^{\text{in}}\right], \end{aligned} \tag{3.87}$$

where

$$\eta^n(\boldsymbol{x}) = \max_{k\in\{0,1,\ldots,n\}} H\big(\rho^k(\boldsymbol{x})\big) \qquad \text{on } \Gamma. \tag{3.88}$$

Note that

$$\eta^n(\boldsymbol{x}) = \eta^{n-1}(\boldsymbol{x}) + \big(H\left(\rho^n(\boldsymbol{x})\right) - \eta^{n-1}(\boldsymbol{x})\big)^+ \qquad \text{on } \Gamma, \tag{3.89}$$

where, as usually, $f^+ := \max(0, f)$. Therefore, the weak form of (3.87) is given by

$$\begin{aligned} &\int_\Omega \left[(\rho^n - \rho^{n-1})\psi + \tau\, \psi\, \boldsymbol{U} \cdot \nabla\rho^n + \tau \nabla\rho^n \cdot \nabla\psi\right] \\ &\qquad + \int_\Gamma (\eta^n - \eta^{n-1})\psi + \tau \int_{\Gamma^{\text{in}}} \rho^n\, \psi\, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| = \tau \int_{\Gamma^{\text{in}}} g\, \psi\, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \end{aligned} \tag{3.90}$$

The following lemma ensures that the problem (3.87) - (3.89) is uniquely solvable provided that $\rho^0 \in H^1(\Omega)$.

Lemma 3.4.22. *Let* $c_0 := \max_{s\in\mathbb{R}} (\mathrm{d}H(s)/\mathrm{d}s)$ *and* $\tau_0 := \min\{1, 2/C_U^2\}$. *If* $\tau < \tau_0$ *and* $\rho^{n-1} \in H^1(\Omega)$ *then* (3.90) *has a unique solution* $\rho^n \in H^1(\Omega)$.

Proof. Define the operator $A(u, v) : H^1(\Omega) \times H^1(\Omega) \to (H^1(\Omega))'$ by

$$\begin{aligned} \langle A(u,v)\,, \psi\rangle = &\int_\Omega v\, \psi\, \mathrm{d}\boldsymbol{x} + \tau \int_\Omega \nabla v \cdot \nabla\psi\, \mathrm{d}\boldsymbol{x} + \int_\Gamma \big(H(v) - \eta^{n-1}\big)^+ \psi\, \mathrm{d}s \\ &+ \tau \int_{\Gamma^{\text{in}}} v\, \psi\, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}|\, \mathrm{d}s - \tau \int_{\Gamma^{\text{in}}} g\, \psi\, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}|\, \mathrm{d}s \\ &+ \tau \int_\Omega \psi\, \boldsymbol{U} \cdot \nabla u\, \mathrm{d}\boldsymbol{x}, \end{aligned} \tag{3.91}$$

where $\psi \in H^1(\Omega)$ is arbitrary, and $\langle\cdot,\cdot\rangle$ denotes the duality product between $(H^1(\Omega))'$ and $H^1(\Omega)$.

We proceed in two steps. Fist, to proof the existence of ρ^n, $n = 1, ..., K$, show that A is of the type of Calculus of Variations (see Definition 3.G.6) and apply Lemma 3.G.7 with $f \in (H^1(\Omega))'$ defined by

$$\langle f\,,\, \psi\rangle = \int_\Omega \rho^{n-1}\, \psi\, \mathrm{d}\boldsymbol{x}.$$

Second, show the uniqueness of ρ^n.

Implementation of Step 1: existence of ρ^n. Proof the conditions of Definition 3.G.6. The boundedness of A follows by applying Hölder's inequality and the embedding $H^1(\Omega) \subset L^4(\partial\Omega)$, $N = 3$, to (3.91):

$$\begin{aligned}\langle A(u,v)\,,\psi\rangle \le \|v\|_{L^2(\Omega)}\;\|\psi\|_{L^2(\Omega)} + \tau\,\|\nabla v\|_{L^2(\Omega)^N}\;\|\nabla\psi\|_{L^2(\Omega)^N}\\ + c_0\|v\|_{L^2(\Gamma)}\,\|\psi\|_{L^2(\Gamma)} + \tau\|v\|^2_{L^4(\Gamma^{\rm in})}\,\|\psi\|^2_{L^4(\Gamma^{\rm in})}\,\|(\boldsymbol{U}_b\cdot\boldsymbol{\nu})\|_{L^2(\Gamma^{\rm in})}\\ + \tau\|g\|_{L^\infty(\Gamma^{\rm in})}\,\|\psi\|_{L^2(\Gamma^{\rm in})}\,\|(\boldsymbol{U}_b\cdot\boldsymbol{\nu})\|_{L^2(\Gamma^{\rm in})}\\ + \tau\,C_U\,\|\psi\|_{L^2(\Omega)}\;\|u\|_{L^2(\Omega)^N}\,.\end{aligned}$$

To estimate the integral over Γ, the following inequality is used

$$\left|\int_\Gamma \big(H(v)-\eta^{n-1}\big)^+\,\psi\,\mathrm{d}s\right| \le \int_\Gamma |H(v)|\;|\psi|\,\mathrm{d}s \le c_0\int_\Gamma |v|\;|\psi|\,\mathrm{d}s.$$

To establish the first property of Definition 3.G.6, show first, that A is hemi-continuous with respect to v. Let $w \in H^1(\Omega)$ be fixed and $\lambda \in \mathbb{R}$, then

$$\begin{aligned}&\left|\int_\Gamma \Big[\big(H(v+\lambda w)-\eta^{n-1}\big)^+ - \big(H(v)-\eta^{n-1}\big)^+\Big]\,\psi\,\mathrm{d}s\right|^2\\ &\quad\le C_\Omega^2\,\|\psi\|^2_{H^1(\Omega)}\cdot\int_\Gamma \left|\big(H(v+\lambda w)-\eta^{n-1}\big)^+ - \big(H(v)-\eta^{n-1}\big)^+\right|^2\mathrm{d}s\end{aligned} \tag{3.92}$$

by Hölder's inequality and the embedding $H^1(\Omega) \subset L^2(\partial\Omega)$. Split the last integral in (3.92) into integrals over the sets

$$\begin{aligned}G_1 &= \{H(v) > \eta^{n-1} \quad\wedge\quad H(v+\lambda w) > \eta^{n-1}\},\\ G_2 &= \{H(v) < \eta^{n-1} \quad\wedge\quad H(v+\lambda w) > \eta^{n-1}\},\\ G_3 &= \{H(v) < \eta^{n-1} \quad\wedge\quad H(v+\lambda w) < \eta^{n-1}\},\\ G_4 &= \{H(v) > \eta^{n-1} \quad\wedge\quad H(v+\lambda w) < \eta^{n-1}\},\end{aligned}$$

then the integral over G_1 can be estimated by

$$\begin{aligned}&\int_{G_1}\left|\big(H(v+\lambda w)-\eta^{n-1}\big)^+ - \big(H(v)-\eta^{n-1}\big)^+\right|^2\mathrm{d}s\\ &\quad\le \int_{G_1} |H(v+\lambda w)-H(v)|^2\,\mathrm{d}s\\ &\quad\le c_0^2\lambda^2\int_{G_1}|w|^2\,\mathrm{d}s.\end{aligned} \tag{3.93}$$

The integral over G_2 can be estimated by

$$\begin{aligned}&\int_{G_2}\left|\big(H(v+\lambda w)-\eta^{n-1}\big)^+ - \big(H(v)-\eta^{n-1}\big)^+\right|^2\mathrm{d}s\\ &\quad= \int_{G_2}\left|\big(H(v+\lambda w)-\eta^{n-1}\big)^+\right|^2\,\mathrm{d}s\\ &\quad\le \int_{G_2}|H(v+\lambda w)-H(v)|^2\,\mathrm{d}s\\ &\quad\le \int_{G_2} c_0^2\,\lambda^2\,|w|^2\,\mathrm{d}s.\end{aligned}$$

The integral over G_3 vanishes, and the integral over G_4 is being estimated by

$$\begin{aligned}
&\int_{G_4} \left| \big(H(v+\lambda w) - \eta^{n-1}\big)^+ - \big(H(v) - \eta^{n-1}\big)^+ \right|^2 \mathrm{d}s \\
&\quad = \int_{G_4} \left| \big(H(v) - \eta^{n-1}\big)^+ \right|^2 \mathrm{d}s \\
&\quad \leq \int_{G_4} |H(v) - H(v+\lambda w)|^2 \, \mathrm{d}s \\
&\quad \leq \int_{G_2} c_0^2 \, \lambda^2 \, |w|^2 \, \mathrm{d}s.
\end{aligned} \tag{3.94}$$

Substituting (3.93) - (3.94) into (3.92) shows that A is hemi-continuous with respect to v.

Show next the inequality in the first property Definition 3.G.6. For $u, v \in H^1(\Omega)$, it holds

$$\begin{aligned}
&\langle A(u,u) - A(u,v) \,,\, (u-v) \rangle \\
&= \int_\Omega |u-v|^2 \, \mathrm{d}\boldsymbol{x} + \tau \int_\Omega |\nabla(u-v)|^2 \mathrm{d}\boldsymbol{x} + \tau \int_{\Gamma^{\mathrm{in}}} |u-v|^2 |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\
&+ \int_\Gamma \left[\big(H(u) - \eta^{n-1}\big)^+ - \big(H(v) - \eta^{n-1}\big)^+ \right] (u-v) \mathrm{d}s \\
&\geq 0,
\end{aligned} \tag{3.95}$$

because $\big(H(u) - \eta^{n-1}\big)^+ - \big(H(v) - \eta^{n-1}\big)^+$ and $(u-v)$ have the same sign and because of (3.83). Therefore, A satisfies the first property of Definition 3.G.6. Clearly, A is hemi-continuous with respect to u. Thus, the second property of Definition 3.G.6 is verified.

To show the third property, assume $u_j \rightharpoonup u$ weakly in $H^1(\Omega)$ and assume that

$$\langle A(u_j, u_j) - A(u_j, u) \,,\, (u_j - u) \rangle \to 0.$$

This implies that $u_j \to u$ strongly in $H^1(\Omega)$. To proof that, replace u by u_j and v by u in (3.95). By Hölder's inequality, the following estimate holds:

$$\begin{aligned}
|\langle A(u_j, v) - A(u,v) \,,\, \psi \rangle| &= \tau \left| \int_\Omega \nabla(u_j - u) \cdot \boldsymbol{U} \, \psi \, \mathrm{d}\boldsymbol{x} \right| \\
&\leq \tau \, C_U \, \|\psi\|_{L^2(\Omega)} \, \|\nabla(u_j - u)\|_{L^2(\Omega)^N} \,.
\end{aligned}$$

The right-hand side tends to 0, which proves the third property of Definition 3.G.6.

To obtain the fourth property, assume that $u_j \rightharpoonup u$ weakly in $H^1(\Omega)$ and assume that $A(u_j, v) \rightharpoonup \phi$ in $(H^1(\Omega))'$. Then

$$\begin{aligned}
\langle A(u_j, v) \,,\, \psi \rangle = &\int_\Omega [v \, \psi + \tau \nabla v \cdot \nabla \psi] \, \mathrm{d}\boldsymbol{x} + \int_\Gamma \big(H(v) - \eta^{n-1}\big)^+ \psi \, \mathrm{d}s \\
&+ \tau \int_{\Gamma^{\mathrm{in}}} v \, \psi \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s - \tau \int_{\Gamma^{\mathrm{in}}} g \, \psi \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\
&+ \tau \int_\Omega \psi \, \boldsymbol{U} \cdot \nabla u_j \, \mathrm{d}\boldsymbol{x}.
\end{aligned}$$

Since u_j appears in the last term only, passing to the limit yields

$$\begin{aligned}\langle \phi\,,\,\psi\rangle = &\int_\Omega [v\,\psi + \tau\nabla v\cdot\nabla\psi]\,\mathrm{d}\boldsymbol{x} + \int_\Gamma \left(H(v)-\eta^{n-1}\right)^+\psi\,\mathrm{d}s\\ &+\tau\int_{\Gamma^{\text{in}}} v\,\psi\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s - \tau\int_{\Gamma^{\text{in}}} g\,\psi\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\\ &+\tau\int_\Omega \psi\,\nabla u\cdot\boldsymbol{U}\,\mathrm{d}\boldsymbol{x},\end{aligned}$$

and we get

$$\begin{aligned}&\langle A(u_j,v)\,,\,u_j\rangle - \langle\phi\,,\,u\rangle\\ &= \int_\Omega v\,(u_j-u)\,\mathrm{d}\boldsymbol{x} + \tau\int_\Omega \nabla v\cdot\nabla(u_j-u)\mathrm{d}\boldsymbol{x}\\ &+\int_\Gamma \left(H(v)-\eta^{n-1}\right)^+(u_j-u)\,\mathrm{d}s,\\ &+\tau\int_{\Gamma^{\text{in}}} v\,(u_j-u)\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s - \tau\int_{\Gamma^{\text{in}}} g\,(u_j-u)\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\\ &+\tau\int_\Omega (u_j-u)\,\boldsymbol{U}\cdot\nabla u_j\,\mathrm{d}\boldsymbol{x} + \tau\int_\Omega u\,\boldsymbol{U}\cdot\nabla(u_j-u)\,\mathrm{d}\boldsymbol{x}.\end{aligned} \tag{3.96}$$

Note that all terms on the right-hand side of (3.96) are linear with respect to u_j except for $\int(u_j-u)\,\boldsymbol{U}\cdot\nabla u_j$. Thus, the assumption $u_j \rightharpoonup u$ weakly in $H^1(\Omega)$ implies that all terms tend to zero as $j\to\infty$ except for (possibly) $\int(u_j-u)\,\boldsymbol{U}\cdot\nabla u_j$. To treat this term, assume that $\int(u_j-u)\,\boldsymbol{U}\cdot\nabla u_j \not\to 0$. Then, there exists $\delta>0$ and a subsequence $\{u_k\}$ of $\{u_j\}$ such that

$$\left|\int_\Omega (u_k-u)\,\boldsymbol{U}\cdot\nabla u_k\,\mathrm{d}\boldsymbol{x}\right| > \delta \qquad \forall k.$$

Due to $H^1(\Omega)\subset\subset L^4(\Omega)$, $N=3$, we can assume that $\{u_k\}$ converges strongly in $L^4(\Omega)$. The limit is u. Hölder's inequality and the assumption (3.83) yield the inequalities

$$0<\delta<\left|\int_\Omega (u_k-u)\,\boldsymbol{U}\cdot\nabla u_k\,\mathrm{d}\boldsymbol{x}\right| \le \|u_k-u\|_{L^4(\Omega)}\cdot\|\boldsymbol{U}\|_{L^4(\Omega)^N}\cdot\|\nabla u_k\|_{L^2(\Omega)^N}\,. \tag{3.97}$$

The the first factor on the right-hand side of (3.97) tends to zero as $k\to\infty$ due to the choice of $\{u_k\}$. The last factor is bounded because $u_k \rightharpoonup u$ weakly in $H^1(\Omega)$. Thus, the right-hand side of (3.97) tends to zero as $k\to\infty$ which is impossible. Therefore $\int(u_j-u)\,\boldsymbol{U}\cdot\nabla u_j \not\to 0$ cannot hold, and equation (3.96) yields $\langle A(u_j,v),\,u_j\rangle \to \langle\phi,\,u\rangle$ as $j\to\infty$. All properties of Definition 3.G.6 are satisfied.

Implementation of Step 2: uniqueness of ρ^n. Assume there are two solutions ρ_1^n and ρ_2^n and set $\bar\rho=\rho_1^n-\rho_2^n$, then

$$\begin{aligned}0 &= \langle A(\rho_1^n)-A(\rho_2^n)\,,\,\rho_1^n-\rho_2^n\rangle\\ &= \int_\Omega |\bar\rho|^2\,\mathrm{d}\boldsymbol{x} + \tau\int_\Omega \left[|\nabla\bar\rho|^2 + \bar\rho\,\boldsymbol{U}\cdot\nabla\bar\rho\right]\mathrm{d}\boldsymbol{x}\\ &+\int_\Gamma \left[\left(H(\rho_1^n)-\eta^{n-1}\right)^+ - \left(H(\rho_1^n)-\eta^{n-1}\right)^+\right]\bar\rho\,\mathrm{d}s\\ &+\tau\int_{\Gamma^{\text{in}}} |\bar\rho|^2\,(\boldsymbol{U}_b\cdot\boldsymbol{\nu})\,\mathrm{d}s.\end{aligned} \tag{3.98}$$

As before, the boundary integrals in (3.98) are nonnegative. Application of Young's inequality to the term $\bar{\rho}\,\boldsymbol{U}\cdot\nabla\bar{\rho}$, together with (3.83), yields

$$\begin{aligned}\int_\Omega |\bar{\rho}|^2\,\mathrm{d}\boldsymbol{x} + \tau\int_\Omega |\nabla\bar{\rho}|^2\,\mathrm{d}\boldsymbol{x} + \tau\int_{\Gamma^{\mathrm{in}}} |\bar{\rho}|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s \\ \le \tau\,\frac{C_U^2}{2}\int_\Omega |\bar{\rho}|^2\,\mathrm{d}\boldsymbol{x} + \frac{\tau}{2}\int_\Omega |\nabla\bar{\rho}|^2\,\mathrm{d}\boldsymbol{x}.\end{aligned} \tag{3.99}$$

Assume $\tau < \min\{1, 2/C_U^2\}$. Then (3.99) yields $\bar{\rho} = 0$. □

3.4.2.2 A priori estimates

Lemma 3.4.23. *Let τ_0 be defined as in Lemma 3.4.22, and ρ_n, $n = 1,...,K$, be a sequence of weak solutions defined by* (3.90). *Set*

$$B_0 := \int_\Omega |\rho^0|^2\,\mathrm{d}\boldsymbol{x} + T\int_{\Gamma^{\mathrm{in}}} |g|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s.$$

Then, it holds

$$\int_\Omega |\rho^j|^2 + \sum_{n=1}^K\int_\Omega |\rho^n-\rho^{n-1}|^2 + \tau\sum_{n=1}^K\left[\int_{\Gamma^{\mathrm{in}}} |\rho^n|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \int_\Omega |\nabla\rho^n|^2\right] \le B_0,$$

for all $j = 1,...,K$, provided $\tau\in(0,\tau_0)$.

Proof. Choose $\psi = \rho^n$ in (3.90) and rewrite the first term as

$$(\rho^n-\rho^{n-1})\rho^n = \frac{1}{2}\left[|\rho^n|^2 + |\rho^n-\rho^{n-1}|^2 - |\rho^{n-1}|^2\right]. \tag{3.100}$$

The term $\rho^n\boldsymbol{U}$ can be estimated by Young's inequality 3.A.1, and the boundedness of $\boldsymbol{U}$ by

$$\left|\int_\Omega \rho^n\,\boldsymbol{U}\nabla\rho^n\right| \le \frac{C_U^2}{2}\,\|\rho^n\|^2_{L^2(\Omega)^N} + \frac{1}{2}\,\|\nabla\rho^n\|_{L^2(\Omega)^N}. \tag{3.101}$$

The integral over Γ is positive. Indeed, (3.89) shows that $\eta^n - \eta^{n-1}\ge 0$. Due to the assumption $\eta^0\ge 0$ in (3.81) and (3.88), it holds: $\eta^n(\boldsymbol{x}) - \eta^{n-1}(\boldsymbol{x}) = 0$ if $\rho^n(\boldsymbol{x})\le 0$.

The integral over $|\rho^n|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|$ is positive, and the right-hand side can be estimated by

$$\left|\int_{\Gamma^{\mathrm{in}}} g\rho^n|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\right| \le \frac{1}{2}\int_{\Gamma^{\mathrm{in}}} |g|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \frac{1}{2}\int_{\Gamma^{\mathrm{in}}} |\rho^n|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|. \tag{3.102}$$

Substituting (3.100), (3.101) and (3.102) into (3.90) and summing up for $n = 1,...,k$ yield

$$\begin{aligned}&\frac{1}{2}\int_\Omega |\rho^k|^2 + \frac{1}{2}\sum_{n=1}^k\int_\Omega |\rho^n-\rho^{n-1}|^2 \\ &\quad + \frac{\tau}{2}\sum_{n=1}^k\left[\int_{\Gamma^{\mathrm{in}}} |\rho^n|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \int_\Omega |\nabla\rho^n|^2\right] \\ &\quad \le \frac{1}{2}\int_\Omega |\rho^0|^2 + \frac{\tau\,k}{2}\int_{\Gamma^{\mathrm{in}}} |g|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|.\end{aligned}$$

This proves the lemma. □

The assumption that the mass flux $g|\boldsymbol{U}_b \cdot \boldsymbol{\nu}|$ through the inlet being time independent is used in the proof of the next lemma.

Lemma 3.4.24. *Let τ_0 be defined as in Lemma 3.4.22, and ρ_n, $n = 1, ..., K$, be a sequence of weak solutions of* (3.90)*. Then, there exists a constant B_1 depending only on g, $\boldsymbol{U}$, and ρ^0 such that*

$$\begin{aligned}&\int_\Omega |\nabla\rho^j|^2 \,\mathrm{d}\boldsymbol{x} + \int_{\Gamma^{\text{in}}} |\rho^j|^2 \,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| \,\mathrm{d}s\\ &\quad + \sum_{n=1}^K \tau \int_\Omega \left[\left|\frac{\rho^n-\rho^{n-1}}{\tau}\right|^2 + |\Delta\rho^n|^2\right]\mathrm{d}\boldsymbol{x}\\ &\quad + \sum_{n=1}^K \left[\int_\Omega |\nabla\rho^n - \nabla\rho^{n-1}|^2 \,\mathrm{d}\boldsymbol{x} + \int_{\Gamma^{\text{in}}} |\rho^n-\rho^{n-1}|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\right] \le B_1\end{aligned}$$

for all $j = 1, ..., K$, provided $\tau \in (0, \tau_0)$.

Proof. Substitute $\psi = \rho^n - \rho^{n-1}$ into (3.90) and use (3.100) with ρ^n and ρ^{n-1} replaced by $\nabla\rho^n$ and $\nabla\rho^{n-1}$, respectively, to obtain

$$\begin{aligned}&\int_\Omega |\rho^n-\rho^{n-1}|^2 + \int_\Gamma (\eta^n-\eta^{n-1})(\rho^n-\rho^{n-1})\\ &\quad + \frac{\tau}{2}\int_\Omega \left[|\nabla\rho^n|^2 + |\nabla\rho^n-\nabla\rho^{n-1}|^2 - |\nabla\rho^{n-1}|^2\right]\\ &\quad + \frac{\tau}{2}\int_{\Gamma^{\text{in}}} \left[|\rho^n|^2 + |\rho^n-\rho^{n-1}|^2 - |\rho^{n-1}|^2\right]|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\\ &\quad = \tau\int_{\Gamma^{\text{in}}} g(\rho^n-\rho^{n-1})|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\\ &\quad + \tau\int_\Omega (\rho^n-\rho^{n-1})\boldsymbol{U}\cdot\nabla\rho^n.\end{aligned} \tag{3.103}$$

The integral over Γ is positive, because $\rho^n(\boldsymbol{x}) \ge \rho^{n-1}(\boldsymbol{x})$ implies $\eta^n(\boldsymbol{x}) \ge \eta^{n-1}(\boldsymbol{x})$, and $\rho^n(\boldsymbol{x}) \le \rho^{n-1}(\boldsymbol{x})$ implies $\eta^n(\boldsymbol{x}) = \eta^{n-1}(\boldsymbol{x})$. The last integral can be estimated using (3.83) and Young's inequality as follows

$$\begin{aligned}&\left|\tau\int_\Omega (\rho^n-\rho^{n-1})\nabla\rho^n\cdot\boldsymbol{U}\right|\\ &\qquad \le \frac{1}{2}\left\|\rho^n-\rho^{n-1}\right\|^2_{L^2(\Omega)} + \frac{\tau^2 C_U^2}{2}\left\|\nabla\rho^n\right\|^2_{L^2(\Omega)^N}.\end{aligned} \tag{3.104}$$

Substituting (3.104) into (3.103) and dividing by τ yields

$$\begin{aligned}&\frac{\tau}{2}\int_\Omega \left|\frac{\rho^n-\rho^{n-1}}{\tau}\right|^2 + \frac{1}{2}\int_\Omega \left[|\nabla\rho^n|^2 + |\nabla\rho^n-\nabla\rho^{n-1}|^2 - |\nabla\rho^{n-1}|^2\right]\\ &\quad + \frac{1}{2}\int_{\Gamma^{\text{in}}} \left[|\rho^n|^2 + |\rho^n-\rho^{n-1}|^2 - |\rho^{n-1}|^2\right]|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\\ &\quad \le \int_{\Gamma^{\text{in}}} g(\rho^n-\rho^{n-1})|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \frac{\tau C_U^2}{2}\left\|\nabla\rho^n\right\|^2_{L^2(\Omega)^N}.\end{aligned} \tag{3.105}$$

Remember that $g|\boldsymbol{U}_b \cdot \boldsymbol{\nu}|$ is assumed to be time independent. Summing up inequality (3.105) for $n = 1, ..., k$ and using B_0 defined in Lemma 3.4.23 to estimate the last term, we obtain

$$\begin{aligned}
&\sum_{n=1}^{k} \frac{\tau}{2} \int_\Omega \left| \frac{\rho^n - \rho^{n-1}}{\tau} \right|^2 \\
&\quad + \frac{1}{2} \sum_{n=1}^{k} \left[\int_\Omega |\nabla\rho^n - \nabla\rho^{n-1}|^2 + \int_{\Gamma^{\text{in}}} |\rho^n - \rho^{n-1}|^2 \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \right] \\
&\quad + \frac{1}{2} \int_\Omega |\nabla\rho^k|^2 + \frac{1}{2} \int_{\Gamma^{\text{in}}} |\rho^k|^2 \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \\
&\quad \leq \frac{1}{2} \int_\Omega |\nabla\rho^0|^2 + \frac{1}{2} \int_{\Gamma^{\text{in}}} |\rho^0|^2 |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| + \frac{C_U^2 \, B_0}{2} \\
&\quad + \int_{\Gamma^{\text{in}}} g \, (\rho^k - \rho^0) \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}|.
\end{aligned} \tag{3.106}$$

Using Young's inequality in the last term of (3.106) and multiplying by 2, we get

$$\begin{aligned}
&\sum_{n=1}^{k} \tau \int_\Omega \left| \frac{\rho^n - \rho^{n-1}}{\tau} \right|^2 \\
&\quad + \sum_{n=1}^{k} \left[\int_\Omega |\nabla\rho^n - \nabla\rho^{n-1}|^2 + \int_{\Gamma^{\text{in}}} |\rho^n - \rho^{n-1}|^2 \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \right] \\
&\quad + \int_\Omega |\nabla\rho^k|^2 + \frac{1}{2} \int_{\Gamma^{\text{in}}} |\rho^k|^2 \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \\
&\quad \leq \int_\Omega |\nabla\rho^0|^2 + \frac{3}{2} \int_{\Gamma^{\text{in}}} |\rho^0|^2 |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| + C_U^2 \, B_0 \\
&\quad + \int_{\Gamma^{\text{in}}} |g|^2 |\boldsymbol{U}_b \cdot \boldsymbol{\nu}|.
\end{aligned} \tag{3.107}$$

To derive an estimate of $\Delta\rho^n$, restrict $\psi \in \mathcal{D}(\Omega)$ in the weak form (3.90) to obtain

$$\langle \Delta\rho^n ; \psi \rangle = - \int_\Omega \nabla\rho^n \cdot \nabla\psi \, \mathrm{d}\boldsymbol{x} = \int_\Omega \psi \left[\frac{\rho^n - \rho^{n-1}}{\tau} + \boldsymbol{U} \cdot \nabla\rho^n \right],$$

which shows $\Delta\rho^n = (\rho^n - \rho^{n-1})/\tau + \boldsymbol{U} \cdot \nabla\rho^n \in L^2(\Omega)$. If we denote the right-hand side of (3.107) by B_1', then Lemma 3.4.23 yields

$$\sum_{n=1}^{k} \tau \int_\Omega |\Delta\rho^n|^2 \, \mathrm{d}\boldsymbol{x} \leq 2 \sum_{n=1}^{k} \tau \int_\Omega \left[\left| \frac{\rho^n - \rho^{n-1}}{\tau} \right|^2 + C_U^2 |\nabla\rho^n|^2 \right] \leq 2B_1' + 2C_U^2 B_0, \tag{3.108}$$

for all $k = 1, ..., K$. Inequalities (3.107) and (3.108) prove the lemma. □

The next lemma provides estimates of the approximate solutions in $L^\infty(\Omega)$.

Lemma 3.4.25. *Let τ_0 be defined as in Lemma 3.4.22, and ρ_n, $n = 1, ..., K$, be a sequence of weak solutions defined by* (3.90). *Set*

$$B_2 := \max \left\{ \|g\|_{L^\infty(\Gamma^{\text{in}})} \, , \; \left\| \rho^0 \right\|_{L^\infty(\Omega)} \right\},$$

Then, it holds $0 \leq \rho^n(\boldsymbol{x}) \leq B_2$ for all $n = 0, ..., K$, and almost all $\boldsymbol{x} \in \Omega$.

Proof. Choose $\psi = f_b'(\rho^n)$ in (3.90) where f_b is defined for $b > 0$ by

$$f_b(s) = \begin{cases} \frac{1}{2}s^2 & \text{if } s < 0, \\ 0 & \text{if } 0 \le s \le b, \\ \frac{1}{2}(s-b)^2 & \text{if } b < s. \end{cases}$$

In order to prove the lemma, we will show that $b \ge B_2$ implies

$$\left\| f_b'(\rho^n) \right\|_{L^2(\Omega)} = 0 \qquad \text{for all } n = 1, ..., K.$$

Observing that

$$f_b'(s) = \begin{cases} s & \text{if } s < 0, \\ 0 & \text{if } 0 < s < b, \\ s-b & \text{if } b < s, \end{cases}$$

shows that f_b satisfies the hypothesis of Lemma 3.A.5, and $f_b'(\rho^n) \in H^1(\Omega)$ due to Lemmas 3.4.24 and 3.E.5. Moreover, the following identities holds: $\nabla\rho^n \, f_b'(\rho^n) = \nabla f_b'(\rho^n) \, f_b'(\rho^n)$ and $\nabla\rho^n \cdot \nabla f_b'(\rho^n) = |\nabla f_b'(\rho^n)|^2$ almost everywhere in Ω. Thus, $f_b'(\rho^n)$ is an admissible testfunction and we obtain from (3.90):

$$\begin{aligned} &\int_\Omega \left[(\rho^n - \rho^{n-1}) f_b'(\rho^n) + \tau |\nabla f_b'(\rho^n)|^2 \right] \\ &\quad + \int_\Gamma (\eta^n - \eta^{n-1}) f_b'(\rho^n) \\ &\quad = \tau \int_{\Gamma^{\text{in}}} (g - \rho^n) \; f_b'(\rho^n) \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| - \tau \int_\Omega f_b'(\rho^n) \, \boldsymbol{U} \cdot \nabla f_b'(\rho^n). \end{aligned} \tag{3.109}$$

Using Lemma 3.A.5 and the identity $2 f_b(s) = f_b'(s)^2$, $s \in \mathbb{R}$, the first term on the left-hand side of (3.109) can be estimated from below by

$$\int_\Omega (\rho^n - \rho^{n-1}) f_b'(\rho^n) \ge \int_\Omega \left[f_b(\rho^n) - f_b(\rho^{n-1}) \right] = \frac{1}{2} \int_\Omega \left[f_b'(\rho^n)^2 - f_b'(\rho^{n-1})^2 \right]. \tag{3.110}$$

For the integral over Γ, it holds

$$\int_\Gamma (\eta^n - \eta^{n-1}) \, f_b'(\rho^n) \, \mathrm{d}s \ge 0. \tag{3.111}$$

If $\rho^n(\boldsymbol{x}) < 0$ then $\eta^n(\boldsymbol{x}) = \eta^{n-1}(\boldsymbol{x})$. If $\rho^n(\boldsymbol{x}) \ge 0$ then $f_b'(\rho^n(\boldsymbol{x})) \ge 0$ and $\eta^n(\boldsymbol{x}) \ge \eta^{n-1}(\boldsymbol{x})$.

The integral over Γ^{in} in (3.109) satisfies

$$\int_{\Gamma^{\text{in}}} (g - \rho^n) \, f_b'(\rho^n) \cdot |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \le 0, \qquad \text{for } b > \|g\|_{L^\infty(\Gamma^{\text{in}})}. \tag{3.112}$$

Indeed, if $f_b'(\rho^n(\boldsymbol{x})) < 0$, then $\rho^n(\boldsymbol{x}) < 0$ and $g(\boldsymbol{x}) - \rho^n(\boldsymbol{x}) \ge 0$. If $f_b'(\rho^n(\boldsymbol{x})) > 0$, then $\rho^n(\boldsymbol{x}) > b \ge g(\boldsymbol{x})$ and $g(\boldsymbol{x}) - \rho^n(\boldsymbol{x}) < 0$.

Using (3.83) and Young's inequality to estimate the last term in (3.109) yields

$$\tau \int_\Omega f_b'(\rho^n) \, \boldsymbol{U} \cdot \nabla f_b'(\rho^n) \le \frac{\tau}{2} \int_\Omega |\nabla f_b'(\rho^n)|^2 + \frac{\tau \, C_U^2}{2} \int_\Omega |f_b'(\rho^n)|^2. \tag{3.113}$$

Substituting (3.110), (3.111), (3.112) and (3.113) into (3.109) and dividing by τ yield

$$\int_\Omega \left[\left(\frac{1}{\tau} - \frac{C_U^2}{2}\right) f_b'(\rho^n)^2 + |\nabla f_b'(\rho^n)|^2\right] \leq \tau \int_\Omega |f_b'(\rho^{n-1})|^2. \tag{3.114}$$

By the hypothesis on τ, it holds: $1/\tau - C_U^2/2 > 0$. Therefore, (3.114) with $n = 1$ yields: $f_b'(\rho^1) = 0$ for $b \geq B_2$. Repeating this argument for $n = 2, ..., K$ proves the lemma. □

To obtain further estimates, define

$$\xi^n(\boldsymbol{x}) := \max_{k\in\{1,...,n\}} \rho^k(\boldsymbol{x}), \qquad \zeta^n(\boldsymbol{x}) := H(\xi^n(\boldsymbol{x})), \qquad \boldsymbol{x} \in \Omega \tag{3.115}$$

and note that ζ^n can be written as

$$\zeta^n(\boldsymbol{x}) := \max_{k\in\{0,1,...,n\}} H(\rho^k(\boldsymbol{x})) = \zeta^{n-1}(\boldsymbol{x}) + \left[H(\rho^n(\boldsymbol{x})) - \zeta^{n-1}(\boldsymbol{x})\right]^+, \quad \boldsymbol{x} \in \Omega.$$

Due to Lemma 3.E.6, we have $\zeta^n \in H^1(\Omega)$, and it holds

$$\eta^n = \gamma_0\, \zeta^n. \tag{3.116}$$

The following lemma gives uniform estimates for ζ^n and η^n.

Lemma 3.4.26. *Let c_0, τ_0 be defined as in Lemma 3.4.22, and ρ^n, $n = 1, ..., K$, be a sequence of weak solutions defined by* (3.90)*. Then, there exists a constant B_3 depending only on g, $\boldsymbol{U}$, and ρ^0 such that*

$$\int_\Omega |\nabla\zeta^j|^2 + \sum_{n=1}^K \left[\tau \int_\Omega \left|\frac{\zeta^n - \zeta^{n-1}}{\tau}\right|^2 + \tau \int_\Gamma \left|\frac{\eta^n - \eta^{n-1}}{\tau}\right|^2 + \int_\Omega \left|\nabla\left(\xi^n - \xi^{n-1}\right)\right|^2\right] \leq B_3$$

for all $j = 1, ..., K$, provided that $\tau \in (0, \tau_0)$.

Proof. Denote $G^n := \{\rho^n \geq \xi^{n-1}\}$ and choose $\psi = \xi^n - \xi^{n-1}$ in (3.90) to obtain

$$\begin{aligned} &\int_\Omega \left[\left(\rho^n - \rho^{n-1}\right)\left(\xi^n - \xi^{n-1}\right) + \tau\nabla\rho^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right)\right] \\ &\quad + \int_\Gamma \left(\eta^n - \eta^{n-1}\right)\left(\xi^n - \xi^{n-1}\right) + \tau\int_{\Gamma^{\text{in}}} \rho^n \left(\xi^n - \xi^{n-1}\right)|\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \\ &\quad = \tau \int_{\Gamma^{\text{in}}} g\left(\xi^n - \xi^{n-1}\right)|\boldsymbol{U}_b \cdot \boldsymbol{\nu}| - \tau\int_\Omega \left(\xi^n - \xi^{n-1}\right)\boldsymbol{U}\cdot\nabla\rho^n. \end{aligned} \tag{3.117}$$

The first term can be estimated from below by

$$\int_\Omega \left(\rho^n - \rho^{n-1}\right)\left(\xi^n - \xi^{n-1}\right) \geq \int_\Omega \left|\xi^n - \xi^{n-1}\right|^2. \tag{3.118}$$

Indeed, if $\boldsymbol{x} \in G^n$, then $\rho^n(\boldsymbol{x}) = \xi^n(\boldsymbol{x})$ and $\xi^n(\boldsymbol{x}) - \rho^{n-1}(\boldsymbol{x}) \geq \xi^n(\boldsymbol{x}) - \xi^{n-1}(\boldsymbol{x}) \geq 0$. If $\boldsymbol{x} \notin G^n$, then $\xi^n(\boldsymbol{x}) = \xi^{n-1}(\boldsymbol{x})$. Similarly, we get for the integral over Γ^{in}:

$$\begin{aligned} \int_{\Gamma^{\text{in}}} \rho^n \left(\xi^n - \xi^{n-1}\right)|\boldsymbol{U}_b \cdot \boldsymbol{\nu}| &= \int_{\Gamma^{\text{in}}} \xi^n \left(\xi^n - \xi^{n-1}\right)|\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \\ &= \frac{1}{2}\int_{\Gamma^{\text{in}}} \left[|\xi^n|^2 - |\xi^n|^2 + \left|\xi^n - \xi^{n-1}\right|^2\right]|\boldsymbol{U}_b \cdot \boldsymbol{\nu}|. \end{aligned} \tag{3.119}$$

Further, $\nabla\rho^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right) = \nabla\xi^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right)$ almost everywhere in Ω. Indeed, $\nabla\left(\xi^n - \xi^{n-1}\right) = \mathbf{0}$ almost everywhere in $\Omega \setminus G^n$, whereas $\rho^n = \xi^n$ and $\nabla\rho^n = \nabla\xi^n$ almost everywhere in G^n. Therefore, we obtain

$$\begin{aligned}\int_\Omega \nabla\rho^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right) &= \int_{G^n} \nabla\rho^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right) \\ &= \int_{G^n} \nabla\xi^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right) = \int_\Omega \nabla\xi^n \cdot \nabla\left(\xi^n - \xi^{n-1}\right) \\ &= \frac{1}{2}\int_\Omega \left[|\nabla\xi^n|^2 - |\nabla\xi^{n-1}|^2 + \left|\nabla\left(\xi^n - \xi^{n-1}\right)\right|^2\right].\end{aligned} \tag{3.120}$$

To estimate the integral over Γ in (3.117) from below, use (3.115) and the Lipschitz-continuity of H to get

$$\zeta^n - \zeta^{n-1} = H(\xi^n) - H(\xi^{n-1}) \le c_0\left(\xi^n - \xi^{n-1}\right). \tag{3.121}$$

Thus, it holds

$$\int_\Gamma \left(\eta^n - \eta^{n-1}\right)\left(\xi^n - \xi^{n-1}\right) \ge \frac{1}{c_0}\int_\Gamma \left|\eta^n - \eta^{n-1}\right|^2. \tag{3.122}$$

To estimate the terms containing $\boldsymbol{U}$ in (3.117), use (3.83) and apply 3.A.1 to obtain

$$\tau\int_\Omega \left(\xi^n - \xi^{n-1}\right)\boldsymbol{U}\cdot\nabla\rho^n \le \frac{C_U^2\,\tau^2}{2}\int_\Omega |\nabla\rho^n|^2 + \frac{1}{2}\int_\Omega \left|\xi^n - \xi^{n-1}\right|^2. \tag{3.123}$$

Substituting (3.118) – (3.123) into (3.117), dividing by τ, summing up for $n = 1, ..., k$, and using the assumption that $g|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|$ is time independent, we get

$$\begin{aligned}&\frac{1}{2}\int_\Omega |\nabla\xi^k|^2 + \frac{1}{2}\int_{\Gamma^{\text{in}}} |\xi^n|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| \\ &+ \sum_{n=1}^k \tau\left[\frac{1}{2}\int_\Omega \left|\frac{\xi^n - \xi^{n-1}}{\tau}\right|^2 + \frac{1}{c_0}\int_\Gamma \left|\frac{\eta^n - \eta^{n-1}}{\tau}\right|^2\right] \\ &+ \frac{1}{2}\sum_{n=1}^k \left[\int_\Omega \left|\nabla\left(\xi^n - \xi^{n-1}\right)\right|^2 + \int_{\Gamma^{\text{in}}} \left|\xi^n - \xi^{n-1}\right|^2 |\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\right] \\ &\le \int_{\Gamma^{\text{in}}} g(\xi^k - \xi^0)|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \frac{C_U^2}{2}\sum_{n=1}^k \tau\int_\Omega |\nabla\rho^n|^2.\end{aligned} \tag{3.124}$$

Taking into account (3.121) and the inequality $|\nabla\zeta^n| = |H'(\xi^n)\nabla\xi^n| \le c_0|\nabla\xi^n|$, applying Young's inequality to the right-hand side of (3.124), and using the constant B_0 defined in Lemma 3.4.23 yield

$$\begin{aligned}&\frac{1}{2c_0^2}\int_\Omega |\nabla\zeta^k|^2 + \frac{1}{4}\int_{\Gamma^{\text{in}}} |\xi^n|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| \\ &+ \sum_{n=1}^k \frac{\tau}{c_0}\left[\frac{1}{c_0}\int_\Omega \left|\frac{\zeta^n - \zeta^{n-1}}{\tau}\right|^2 + \int_\Gamma \left|\frac{\eta^n - \eta^{n-1}}{\tau}\right|^2\right] \\ &+ \frac{1}{2}\sum_{n=1}^k \left[\int_\Omega \left|\nabla\left(\xi^n - \xi^{n-1}\right)\right|^2 + \int_{\Gamma^{\text{in}}} \left|\xi^n - \xi^{n-1}\right|^2 |\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\right] \\ &\le 2\int_{\Gamma^{\text{in}}} |g|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \frac{1}{4}\int_{\Gamma^{\text{in}}} |\rho^0|^2\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| + \frac{C_U^2\,B_0}{2}.\end{aligned}$$

This proves the lemma. □

3.4.2.3 Passage to the limit

For every $K \in \mathbb{N}$ define two kinds of time interpolations of $\{\rho^n\}$, $\{\eta^n\}$, and $\{\zeta^n\}$. Let ρ^K, η^K, ζ^K be piecewise linear interpolations, whereas $\bar{\rho}^K$, $\bar{\eta}^K$, $\bar{\zeta}^K$ are piecewise constant ones. That is

$$\rho_K(\boldsymbol{x},t) = \left(1 - n + \frac{t}{\tau}\right)\rho^n(\boldsymbol{x}) + \left(n - \frac{t}{\tau}\right)\rho^{n-1}(\boldsymbol{x}), \qquad \bar{\rho}_K(\boldsymbol{x},t) = \rho^n(\boldsymbol{x}) \tag{3.125}$$

if $t \in ((n-1)\tau, n\tau]$, $n = 1, ..., K$, and the functions η_K, ζ_K, $\bar{\eta}_K$, and $\bar{\zeta}_K$ are defined in the same way. The following lemma shows in which sense the piecewise linear and piecewise constant interpolations converge to each other.

Lemma 3.4.27. *For $K \to \infty$ the interpolations defined by* (3.125) *satisfy:*

$$\begin{aligned} [\rho_K(t) - \bar{\rho}_K(t)] &\to 0 \qquad \textit{in} \quad L^2(\Omega), \\ [\zeta_K(t) - \overline{\zeta}_K(t)] &\to 0 \qquad \textit{in} \quad L^2(\Omega), \\ [\eta_K(t) - \overline{\eta}_K(t)] &\to 0 \qquad \textit{in} \quad L^2(\Gamma), \end{aligned}$$

and the convergence is uniform for $t \in [0,T]$. Moreover

$$(\rho_K - \bar{\rho}_K) \to 0 \quad \textit{in} \quad L^2(0,T;H^1(\Omega)).$$

Proof. Due to Lemma 3.4.24, the following estimate holds true

$$\begin{aligned} &\int_0^T \left[\|\rho_K(t) - \bar{\rho}_K(t)\|^2_{L^2(\Omega)} + \|\nabla\rho_K(t) - \nabla\bar{\rho}_K(t)\|^2_{L^2(\Omega)}\right] \mathrm{d}t \\ &= \sum_{n=1}^K \left[\left\|\rho^n - \rho^{n-1}\right\|^2_{L^2(\Omega)} + \left\|\nabla\rho^n - \nabla\rho^{n-1}\right\|^2_{L^2(\Omega)}\right] \cdot \int_{(n-1)\tau}^{n\tau} \left(\frac{t}{\tau} - n\right)^2 \mathrm{d}t \\ &\le \frac{\tau}{3}\max\{1,\, \tau\} \left[\sum_{n=1}^K \tau \int_\Omega \left|\frac{\rho^n - \rho^{n-1}}{\tau}\right|^2 \mathrm{d}\boldsymbol{x} + \sum_{n=1}^K \int_\Omega |\nabla\rho^n - \nabla\rho^{n-1}|^2 \,\mathrm{d}\boldsymbol{x}\right], \end{aligned}$$

where the term on the right-hand side in square brackets is bounded by B_1. This proves the last assertion of the lemma, because $\tau = T/K$.

The other assertions of the lemma are obvious for $t = 0$. For each $t \in (0,T]$ and $K \in \mathbb{N}$, we have $(n_K - 1)\tau < t \le n_K\,\tau$ for a certain $n_K \in \{1, ..., K\}$. And therefore, by (3.125):

$$|\rho_K(\boldsymbol{x},t) - \bar{\rho}_K(\boldsymbol{x},t)| = \left(n_K - \frac{t}{\tau}\right) \cdot \tau \cdot \frac{\left|\rho^{n_K-1}(\boldsymbol{x}) - \rho^{n_K}(\boldsymbol{x})\right|}{\tau},$$

where $0 < n_K - t/\tau < 1$. Computing the $L^2(\Omega)$-norm and using Lemma 3.4.24 yield

$$\begin{aligned} \int_\Omega |\rho_K(\boldsymbol{x},t) - \bar{\rho}_K(\boldsymbol{x},t)|^2 \,\mathrm{d}\boldsymbol{x} &\le \tau^2 \int_\Omega \left|\frac{\rho^{n_K-1} - \rho^{n_K}}{\tau}\right|^2 \\ &\le \tau \sum_{n=1}^K \tau \left|\frac{\rho^{n-1} - \rho^n}{\tau}\right|^2 \le \tau\, B_1, \end{aligned}$$

where B_1 is independent of K and t. This proves the first assertion about ρ_K and $\bar{\rho}_K$. The claims concerning ζ_K and $\bar{\zeta}_K$, and η_K and $\bar{\eta}_K$ can be shown in a similar way using Lemma 3.4.26 instead of 3.4.24. □

Lemmas 3.4.24 to 3.4.26 imply

$$\begin{aligned}
&\|\rho_K\|_{L^\infty(\Omega\times(0,T))}\ ,\ \|\bar{\rho}_K\|_{L^\infty(\Omega\times(0,T))} \le B_2,\\
&\|(\rho_K)_t\|_{L^2(\Omega\times(0,T))}\ ,\ \|\Delta\rho_K\|_{L^2(\Omega\times(0,T))} \le B_1,\\
&\|\nabla\rho_K\|_{L^\infty(0,T;L^2(\Omega))}\ ,\ \|\nabla\bar{\rho}_K\|_{L^\infty(0,T;L^2(\Omega))} \le B_1,\\
&\|(\zeta_K)_t\|_{L^2(\Omega\times(0,T))}\ ,\ \|(\eta_K)_t\|_{L^2(\Gamma\times(0,T))} \le B_3,\\
&\|\nabla\zeta_K\|_{L^\infty(0,T;L^2(\Omega))}\ ,\ \|\nabla\bar{\zeta}_K\|_{L^\infty(0,T;L^2(\Omega))} \le B_3.
\end{aligned} \tag{3.126}$$

Moreover, the relation (3.116) and the embedding $H^1(\Omega) \subset H^{1/2}(\partial\Omega)$ yield bounds for the norms

$$\|\eta_K\|_{L^\infty(0,T;H^{1/2}(\Gamma))}\ ,\ \|\bar{\eta}_K\|_{L^\infty(0,T;H^{1/2}(\Gamma))}\ .$$

Therefore, there exist functions

$$\begin{aligned}
&\rho \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T)),\\
&\eta \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^{1/2}(\Gamma)),\\
&\zeta \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T)),
\end{aligned} \tag{3.127}$$

and a subsequence $\{K_m\}_{m\in\mathbb{N}}$ such that the approximations converge as follows

$$\begin{aligned}
\rho_{K_m} &\to \rho \quad *-\text{weakly in} \quad H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T)),\\
\bar{\rho}_{K_m} &\to \rho \quad *-\text{weakly in} \quad L^\infty(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T)),\\
\zeta_{K_m} &\to \zeta \quad *-\text{weakly in} \quad H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T)),\\
\bar{\zeta}_{K_m} &\to \zeta \quad *-\text{weakly in} \quad L^\infty(0,T;H^1(\Omega)) \cap L^\infty(\Omega\times(0,T)),\\
\eta_{K_m} &\to \eta \quad *-\text{weakly in} \quad H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{1/2}(\Gamma)),\\
\bar{\eta}_{K_m} &\to \eta \quad *-\text{weakly in} \quad L^\infty(0,T;H^{1/2}(\Gamma)).
\end{aligned} \tag{3.128}$$

Next, show that ρ and η satisfy (3.86). The equations (3.87), (3.88), under accounting for estimates (3.126), yield:

$$\begin{aligned}
(\rho_K)_t + \boldsymbol{U}\cdot\nabla\bar{\rho}_K &= \Delta\bar{\rho}_K && \text{in } L^2(\Omega\times(0,T)),\\
-\partial_{\boldsymbol{\nu}}\,\bar{\rho}_K &= (\eta_K)_t && \text{in } L^2(0,T;H^{-1/2}(\Gamma)),\\
-\partial_{\boldsymbol{\nu}}\,\bar{\rho}_K &= (\bar{\rho}_K - g)|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| && \text{in } L^2(0,T;H^{-1/2}(\Gamma^{\text{in}})),\\
-\partial_{\boldsymbol{\nu}}\,\bar{\rho}_K &= 0 && \text{in } L^2(0,T;H^{-1/2}(\partial\Omega\setminus[\Gamma\cup\Gamma^{\text{in}}])),\\
\bar{\eta}_K(\boldsymbol{x},t) &= \mathcal{A}(\bar{\rho}_K(\boldsymbol{x},\cdot))(t) && \text{for a.a. } (\boldsymbol{x},t)\in\Gamma\times(0,T),\\
\bar{\zeta}_K(\boldsymbol{x},t) &= \mathcal{A}(\bar{\rho}_K(\boldsymbol{x},\cdot))(t) && \text{for a.a. } (\boldsymbol{x},t)\in\Omega\times(0,T),
\end{aligned} \tag{3.129}$$

and, due to (3.116), it holds

$$\bar{\eta}_K = \gamma_0\, \bar{\zeta}_K \qquad \text{in } L^\infty(0,T;H^{1/2}(\Gamma)). \tag{3.130}$$

In the weak form, (3.129) reads (ρ^n are defined by (3.90)):

$$\begin{aligned} &\int_0^T \int_\Omega [(\rho_K)_t + \boldsymbol{U}\cdot\nabla\bar{\rho}_K]\,\psi\,\mathrm{d}\boldsymbol{x}\mathrm{d}t + \int_0^T \int_\Omega \nabla\bar{\rho}_K\cdot\nabla\psi\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \\ &\quad + \int_0^T \int_\Gamma (\eta_K)_t\,\psi\,\mathrm{d}s\mathrm{d}t + \int_0^T \int_{\Gamma^{\mathrm{in}}} \bar{\rho}_K\,\psi|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\mathrm{d}t \\ &\quad = \int_0^T \int_{\Gamma^{\mathrm{in}}} g\,\psi|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\mathrm{d}t \end{aligned} \tag{3.131}$$

for all $\psi \in L^2(0,T;H^1(\Omega))$.

The passage to the limit with respect to subsequences in (3.129), (3.130) and (3.131) yields

$$\begin{aligned} \rho_t + \boldsymbol{U}\cdot\nabla\rho &= \Delta\rho && \text{in } L^2(\Omega\times(0,T)), \\ -\partial_{\boldsymbol{\nu}}\rho &= \eta_t && \text{in } L^2(0,T;H^{-1/2}(\Gamma)), \\ -\partial_{\boldsymbol{\nu}}\rho &= (\rho - g)\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| && \text{in } L^2(0,T;H^{-1/2}(\Gamma^{\mathrm{in}})), \\ -\partial_{\boldsymbol{\nu}}\rho &= 0 && \text{in } L^2(0,T;H^{-1/2}(\partial\Omega\setminus[\Gamma\cup\Gamma^{\mathrm{in}}])), \\ \eta &= \gamma_0\zeta && \text{in } L^\infty(0,T;H^{1/2}(\Gamma)) \end{aligned} \tag{3.132}$$

so that ρ and η satisfy the weak form (3.86).

Lemma 3.4.28. *Let ρ and ζ be the limits in* (3.127)*,* (3.128)*. Then the following equality holds*

$$\zeta(\boldsymbol{x},t) = \mathcal{A}(\rho(\boldsymbol{x},\cdot))(t) \tag{3.133}$$

for almost all $(\boldsymbol{x},t)\in\Omega\times(0,T)$.

Proof. First, we proof that there exist subsequences, again denoted by $\{\zeta_{K_m}\}$, $\{\bar{\zeta}_{K_m}\}$, which satisfy:

$$\begin{aligned} \zeta_{K_m} &\to \zeta && \text{in } \mathcal{C}(0,T;H^{1-\epsilon}(\Omega)), \\ \zeta_{K_m} &\to \mathcal{A}(\rho) && \text{in } \mathcal{C}(0,T;L^2(\Omega)), \\ \bar{\zeta}_{K_m}(t) &\to \mathcal{A}(\rho)(t) && \text{in } L^2(\Omega), \quad \text{uniformly for } t\in[0,T]. \end{aligned} \tag{3.134}$$

Due to the estimates from (3.126) and Theorem 3.F.2, applied with $X = H^1(\Omega)$, $B = H^{1-\epsilon}(\Omega)$, and $Y = L^2(\Omega)$, there exists a subsequence of (ζ_{K_m}) that convergences in $\mathcal{C}(0,T;H^{1-\epsilon}(\Omega))$. By (3.128), the limit equals ζ, which proves the first assertion of (3.134).

The second assertion can be shown almost in the same way as in [63, IX.1]. Note that the following embedding is true:

$$H^1(\Omega\times(0,T)) \subset\subset L^2(\Omega;\mathcal{C}[0,T]).$$

Therefore, a subsequence, again denoted by ρ_{K_m}, satisfies

$$\rho_{K_m} \to \rho \qquad \text{in } L^2(\Omega;\mathcal{C}[0,T]) \tag{3.135}$$

so that $\rho_{K_m}(\boldsymbol{x},\cdot) \to \rho(\boldsymbol{x},\cdot)$ in $\mathcal{C}[0,T]$ for almost all $\boldsymbol{x} \in \Omega$.

Similar to the proof of Lemma 3.4.27, fix an arbitrary $t \in (0,T]$ and set $\tau := T/K$. Then, there exists an integer $n \in \{1,...,K\}$ such that $(n-1)\tau < t \le n\,\tau$. From (3.115), the definition of $\mathcal{A}$, and the convergence (3.135), it follows

$$\begin{aligned} |\zeta_{K_m}(\boldsymbol{x},t) - \mathcal{A}(\rho(\boldsymbol{x},\cdot))(t)| &= \left| \max_{s\le t} H(\rho_{K_m}(\boldsymbol{x},s)) - \max_{s\le t} H(\rho(\boldsymbol{x},s)) \right| \\ &\le c_0 \max_{s\le t} |\rho_{K_m}(\boldsymbol{x},s) - \rho(\boldsymbol{x},s)| \\ &\le c_0 \, \|\rho_{K_m}(\boldsymbol{x},\cdot) - \rho(\boldsymbol{x},\cdot)\|_{\mathcal{C}[0,T]} \end{aligned}$$

for almost all $\boldsymbol{x} \in \Omega$, where $c_0 = \max \mathrm{d}H(s)/\mathrm{d}s$. Computing the $L^2(\Omega)$-norm of the both sides of the previous relation yields

$$\int_\Omega |\zeta_{K_m}(\boldsymbol{x},t) - \mathcal{A}(\rho(\boldsymbol{x},\cdot))(t)|^2 \, \mathrm{d}\boldsymbol{x} \le c_0^2 \|\rho_{K_m}(\boldsymbol{x},\cdot) - \rho(\boldsymbol{x},\cdot)\|^2_{L^2(\Omega;\,\mathcal{C}[0,T])},$$

where the right-hand side tends to zero independently of t because of (3.135). This proves the second assertion of (3.134).

The third assertion is a consequence of the second one and Lemma 3.4.27.

It is easy to see that the first and second assertions of (3.134) prove the claim of the lemma. □

To proof the existence of solutions to (3.81), it is necessary to establish that $\eta = \mathcal{A}(\gamma_0\rho)$ (see (3.85)). This relation is the consequence of Lemma 3.4.28 and the results of the next section where the commutativity of $\mathcal{A}$ and γ_0 is established.

3.4.2.4 Representation of the trace

We have already shown that ρ and η are related by the identity $\eta = \gamma_0\mathcal{A}(\rho)$ (see (3.132) and (3.133)). However, to show the existence of solutions to problem (3.81) in the sense of Definition 3.4.19, the identity (3.85) has to be established. This identity is also important for the proof of the uniqueness of $(\rho,\,\eta)$ using Hilpert's inequality, see Section 3.4.2.5.

To proof of (3.85), we use regularity results for solutions of elliptic problems in Lipschitz domains (see Theorem 3.4.29) and an anisotropic embedding (see Theorem 3.4.34) that ensures certain continuity properties of $\rho(x,y,z,t)$ in the variables (z,t), if $N = 3$. The following theorem deals with the regularity of solutions to elliptic problems in Lipschitz domains.

Theorem 3.4.29 ([52, Theorem 4]). *Let Ω be a Lipschitz bounded open set, let $\boldsymbol{\nu}$ be the exterior unit normal to its boundary, and let $A(\boldsymbol{x})$ be symmetric matrices with measurable coefficients satisfying*

$$\begin{aligned} &\exists \alpha,\mu > 0 \;:\; \alpha|\boldsymbol{\xi}|^2 \le A(\boldsymbol{x})\boldsymbol{\xi}\cdot\boldsymbol{\xi} \le \mu|\boldsymbol{\xi}|^2, \quad \forall \boldsymbol{\xi} \in \mathbb{R}^N, \quad \text{for a.e. } \boldsymbol{x} \in \Omega, \\ &\exists L > 0 \;:\; |A(\boldsymbol{x}) - A(\boldsymbol{y})| \le L|\boldsymbol{x}-\boldsymbol{y}|, \quad \forall \boldsymbol{x},\, \boldsymbol{y} \in \Omega. \end{aligned}$$

If $f \in L^2(\Omega)$ and $g \in H^{-1/2+s}(\partial\Omega)$, $s \in (-1/2, 1/2)$, then the non-homogeneous Neumann problem:

$$\begin{aligned} -\mathrm{div}\, A(\boldsymbol{x})\nabla u(\boldsymbol{x}) + \lambda u &= f(\boldsymbol{x}) \quad \text{in } \Omega, \\ \partial_{\boldsymbol{\nu}_A} u(\boldsymbol{x}) &= g(\boldsymbol{x}) \quad \text{on } \partial\Omega, \end{aligned}$$

(with $\lambda > 0$ and $\boldsymbol{\nu}_A = A\boldsymbol{\nu}$) admits a unique solution $u \in H^{1+s}(\Omega)$.

Let us note that the proof Theorem 3.4.29 given in [52] yields the following bound for the $H^{1+s}(\Omega)$-norm of u: $\|u\|_{H^{1+s}(\Omega)} \leq C(\|f\|_{L^2(\Omega)} + \|g\|_{H^{-1/2+s}(\partial\Omega)})$.
The result of this section is formulated in the following lemma.

Lemma 3.4.30. *The limits* ρ *and* η *from* (3.128) *satisfy identity* (3.85). *Moreover it holds:* $\rho \in L^2(0,T;H^{3/2-\epsilon}(\Omega))$ *for any* $\epsilon > 0$.

Proof. The proof of the lemma is divided into the following three steps:

1. Show $\rho \in L^2(0,T;H^{3/2-\epsilon}(\Omega))$, for any $\epsilon > 0$.
2. Show $\rho \in L^q((0,X) \times (0,Y); \mathcal{C}([0,Z] \times [0,T]))$, provided that Ω contains the cube $(0,X) \times (0,Y) \times (0,Z)$ where X, Y and Z are positive numbers.
3. Deduce (3.85).

Implementation of Step 1. Remember that Ω is supposed to be a Lipschitz domain. Thus, Theorem 3.4.29 is applicable to elliptic problems in Ω. For almost all $t \in (0,T)$ and any $\lambda > 0$, the function $\rho(t)$ is a solution of the following non-homogeneous Neumann problem

$$\begin{aligned} -\Delta u + \lambda u = f &:= -\rho_t(t) - \boldsymbol{U} \cdot \nabla\rho(t) + \lambda\rho(t) && \text{in } \Omega, \\ \partial_{\boldsymbol{\nu}} u &= q && \text{on } \partial\Omega, \end{aligned} \tag{3.136}$$

where the boundary function q is given by

$$q(\boldsymbol{x}) = \begin{cases} \eta_t(\boldsymbol{x},t) & \boldsymbol{x} \in \Gamma, \\ \big(g(\boldsymbol{x}) - \rho(\boldsymbol{x},t)\big)\ |\boldsymbol{U}_b(\boldsymbol{x}) \cdot \boldsymbol{\nu}| & \boldsymbol{x} \in \Gamma^{\text{in}}, \\ 0 & \boldsymbol{x} \in \partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}}). \end{cases}$$

By the regularity of ρ and η given in (3.127), it holds $q \in L^2(0,T;L^2(\partial\Omega))$. Moreover, the regularity of ρ and the properties of $\boldsymbol{U}$ (see (3.83)), imply $f \in L^2(0,T;L^2(\Omega))$. Thus, Theorem 3.4.29 can be applied to problem (3.136) with $s = 1/2 - \epsilon$ and yields $\rho(t) = u \in H^{3/2-\epsilon}(\Omega)$ for almost all $t \in (0,T)$. Due to the regularity of q and f, it holds $\rho \in L^2(0,T;H^{3/2-\epsilon}(\Omega))$. This completes the proof of Step 1.

Implementation of Step 2. Let Ω contain a cube of the form $(0,X) \times (0,Y) \times (0,Z)$ where X, Y, Z are positive numbers. In order to apply Theorem 3.4.34, we have to find some $p > 2$ such that $\rho_{x_i} \in L^p(\Omega \times (0,T))$ holds. By (3.127) and the following embedding

$$H^{1/2-\epsilon}(\Omega) \subset L^{p_1}(\Omega), \qquad p_1 = \frac{6}{3 - (1/2-\epsilon)\cdot 2} = 3 - \epsilon', \qquad \epsilon' = \frac{3\,\epsilon}{1+\epsilon}, \tag{3.137}$$

we obtain

$$\rho_{x_i} \in L^2(0,T;L^{p_1}(\Omega)) \cap L^\infty(0,T;L^2(\Omega)) \tag{3.138}$$

for $i = 1, ..., N$. Thus, Hölder's inequality yields the following estimate

$$\begin{aligned} \left[\int_0^T \int_\Omega |\rho_{x_i}|^p\right]^{1/p} \leq & \left[\int_0^T \left(\int_\Omega |\rho_{x_i}|^2\right)^{1/(3-p)}\right]^{(3-p)/2} \\ & \times \left[\int_0^T \left(\int_\Omega |\rho_{x_i}|^{2(p-1)}\right)^{1/(p-1)}\right]^{(p-1)/2} \end{aligned}$$

for $p > 1$. Therefore, (3.138) with $p_1 = 2(p-1)$ yields

$$\rho_{x_i} \in L^p(\Omega \times (0,T)), \qquad p = \frac{5}{2} - \frac{\epsilon'}{2}. \tag{3.139}$$

Taking into account the regularity of ρ given by (3.127) and (3.139), and applying Theorem 3.4.34 we obtain

$$\rho \in L^q((0,X) \times (0,Y)\,; \mathcal{C}([0,Z] \times [0,T])), \qquad \text{if} \qquad p \le q < \frac{2(p+2)}{6-p}. \tag{3.140}$$

Note that such q exist for sufficiently small ϵ because of inequality (3.166) and because $p > 2$ for $\epsilon' \in (0,1)$, see (3.139) and (3.137). This completes the proof of Step 2.

Implementation of Step 3. Let X, Y, and Z be the numbers from the previous step, and let us assume for simplicity that $\Gamma = (0,X) \times (0,Y) \times \{0\}$. Denote by $\Gamma_N = (0,X) \times (0,Y)$ the projection of Γ onto the hyperplane $\{\boldsymbol{x} : x_N = 0\}$, then (3.140) can be rewritten as $\rho \in L^q(\Gamma_N\,; \mathcal{C}([0,Z] \times [0,T]))$. According to [2, A 6.6] the trace $\gamma_0\, u$ on Γ of function $u \in H^1(\Omega)$ is defined by

$$\gamma_0\, u(\boldsymbol{x}) = \lim_{z \to 0+} u(\boldsymbol{x} + z\,\boldsymbol{e}_N),$$

and it is shown that $\int_\Gamma |\gamma_0\, u(\boldsymbol{x}) - u(\boldsymbol{x} + z\,\boldsymbol{e}_N)|^2 \mathrm{d}s \to 0$.

Remember that $\eta = \gamma_0 \mathcal{A}(\rho)$ is already shown. Therefore, $\eta = \mathcal{A}(\gamma_0\, \rho)$ is proved if we can show that

$$|\mathcal{A}(\rho(x,y,0,\cdot))(t) - \mathcal{A}(\rho(x,y,z,\cdot))(t)| \to 0 \qquad \text{as } z \to 0+ \tag{3.141}$$

for all $t \in [0,T]$ with $\mathcal{A}(\rho)(t) \in H^1(\Omega)$ and for almost all $(x,y) \in \Gamma_N$. Suppose $N = 3$. For almost all $(x,y) \in \Gamma_N$, the function $\rho(x,y,z,s)$ is continuous in the variables (z,s) (see (3.140)). Thus, it is uniformly continuous on compact sets of the form $(z,s) \in [0,Z] \times [0,T]$. Fix an arbitrary t for which $\mathcal{A}(\rho)(t) \in H^1(\Omega)$. Then, for almost all $(x,y) \in \Gamma^N$, the following estimate holds true

$$\begin{aligned} |\mathcal{A}(\rho(x,y,0,\cdot))(t) - \mathcal{A}(\rho(x,y,z,\cdot))(t)| &= \left| \max_{s \le t} \rho(x,y,0,s) - \max_{s \le t} \rho(x,y,z,s) \right| \\ &\le \max_{s \le t} |\rho(x,y,0,s) - \rho(x,y,z,s)|\,. \end{aligned} \tag{3.142}$$

The right-hand side of (3.142) tends to zero as $z \to 0+$ due to the uniform continuity of $\rho(x,y,\cdot,\cdot)$. Thus, (3.141) holds, and we obtain $\gamma_0 \mathcal{A}(\rho)(t) = \mathcal{A}(\gamma_0\, \rho)(t)$ for almost all $t \in (0,T)$. Finally, taking into account the last equation in (3.132) and Lemma 3.4.28, we obtain the following equalities

$$\eta(t) = \gamma_0\, \zeta(t) = \gamma_0\, \mathcal{A}(\rho)(t) = \mathcal{A}(\gamma_0\, \rho)(t)$$

for almost all $t \in (0,T)$. This completes the proof of Step 3. □

3.4.2.5 Uniqueness

To complete the proof of Theorem 3.4.21, it remains to show the uniqueness of solutions to problem (3.81) if the velocity field $\boldsymbol{U}$ satisfies (3.84). To this end, Hilpert's inequality (see Theorem 3.C.1) is used. The following remark provides some preparations.

Remark 3.4.31. *1. Note that the functions γ_l and γ_r (see Section 3.C) corresponding to the hysteresis operator $\mathcal{A}$ (see* (3.82) *and Figure 2.5.3) are given by*

$$\gamma_l,\, \gamma_r : \mathbb{R} \to [0,1], \qquad \gamma_l(s) \equiv 1, \qquad \gamma_r(s) = H(s).$$

These functions satisfy the conditions (3.175)*.*

2. *Theorem 3.C.1 is not directly applicable because the regularity of ρ given by* (3.127) *and Lemma 3.4.30 does not imply a boundary regularity of the form: $\rho(\boldsymbol{x},\cdot) \in W^{1,1}(0,T)$ a.e. in Γ. However, note that the proof of Theorem 3.C.1 given in [63] is based on the following property: $\sigma \in W^{1,1}(0,T)$ implies $\epsilon = \mathcal{E}(\sigma,\, \epsilon^0) \in W^{1,1}(0,T)$, where $\mathcal{E}$ denotes a play operator under consideration. The proof remains correct without changes if the assumption $(\sigma_i, \epsilon^0) \in W^{1,1}[0,T] \times \mathbb{R}$, $i = 1,2$ is replaced by the following assumption:*

$$(\sigma_i,\, \epsilon^0,\, \epsilon_i) \in \mathcal{C}[0,T] \times \mathbb{R} \times W^{1,1}(0,T), \quad \textit{where } \epsilon_i = \mathcal{E}(\sigma_i,\, \epsilon^0) \quad (i = 1,2). \quad (3.143)$$

Let us show that the functions ρ and η satisfy (3.143) *almost everywhere in Γ. It holds: $\eta = \mathcal{A}(\gamma_0\, \rho) \in L^2(\Gamma;\, H^1(0,T))$ due to Lemma 3.4.30 and the regularity of η given in* (3.127)*. Thus, we obtain $\mathcal{A}(\rho(\boldsymbol{x},\cdot)) \in W^{1,1}(0,T)$ for almost all $\boldsymbol{x} \in \Gamma$. Moreover, the regularity result* (3.140) *implies that $\rho(\boldsymbol{x},\cdot) \in \mathcal{C}([0,T])$ for almost all $\boldsymbol{x} \in \Gamma$. Consequently, the requirement* (3.143) *is satisfied almost everywhere in Γ if $(\sigma_i,\, \epsilon_i,\, \mathcal{E})$ is replaced by $(\rho_i(\boldsymbol{x},\cdot),\, \eta_i(\boldsymbol{x},\cdot),\, \mathcal{A})$, $i = 1,2$.*

3. *To apply Hilpert's inequality, terms of the form $\phi\, \boldsymbol{U} \cdot \nabla\psi$ have to be integrated by parts. If $\phi,\, \psi \in H^1(\Omega)$, and $\boldsymbol{U}$ satisfies* (3.83)*, estimate the $H^1(\Omega)^N$-norm of $\phi\, \boldsymbol{U}$, then use the weak Gaussian Theorem 3.E.4.*

   By (3.83)*, it holds: $\phi\, \boldsymbol{U} \in L^2(\Omega)^N$. To show that $\nabla(\phi\, \boldsymbol{U}) \in L^2(\Omega)^{N\times N}$, let U be an arbitrary component of $\boldsymbol{U}$. The product rule yields $\nabla(\phi\, U) = U\, \nabla\phi + \phi\, \nabla U \in L^1(\Omega)$. Due to* (3.83) *and the embedding $H^{1/2+\epsilon}(\Omega)^N \subset L^3(\Omega)$, $N = 3$, we have $\nabla U(t) \in L^3(\Omega)$, $t \in [0,T]$. Accounting for* (3.83) *and using Hölder's inequality, the following estimates show that $\nabla(\phi\, U) \in L^2(\Omega)^N$:*

$$\int_\Omega |U\, \nabla\phi|^2 \le C_U^2 \int_\Omega |\nabla\phi|^2, \qquad \int_\Omega |\phi\, \nabla U|^2 \le \|\phi\|^2_{L^6(\Omega)} \cdot \|\nabla U\|^2_{L^3(\Omega)^N} \,.$$

   Therefore, Theorem 3.E.4 yields

$$\int_\Omega \phi\, \boldsymbol{U} \cdot \nabla\psi + \int_{\Gamma^{\mathrm{in}}} \phi\, \psi |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| = \int_\Omega \psi\, [\phi\, \mathrm{div}\, \boldsymbol{U} + \boldsymbol{U} \cdot \nabla\phi] + \int_{\Gamma^{\mathrm{out}}} \phi\, \psi |\boldsymbol{U}_b \cdot \boldsymbol{\nu}|,$$

   by the properties of $\boldsymbol{U}$ on the boundary (see (3.83)*).*

The following lemma states the result of this section.

Lemma 3.4.32. *Let the velocity field $\boldsymbol{U}$ satisfy* (3.84)*. Then, the limits ρ and η given by* (3.128) *are unique weak solutions of problem* (3.81)*.*

Proof. Let $(\rho_i,\, \eta_i)$, $i = 1,2$, be two solutions to problem (3.81). Define $\bar\rho := \rho_1 - \rho_2$ and $\bar\eta := \eta_1 - \eta_2$. By (3.86), $\bar\rho$, $\bar\eta$ satisfy the following integral identity

$$\int_0^T \int_\Omega [\bar\rho_t + \boldsymbol{U} \cdot \nabla\bar\rho]\, \psi + \int_0^T \int_\Omega \nabla\bar\rho \cdot \nabla\psi + \int_0^T \int_\Gamma \bar\eta_t\, \psi + \int_0^T \int_{\Gamma^{\mathrm{in}}} \bar\rho\, \psi |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| = 0$$

for any $\psi \in L^2(0,T;H^1(\Omega))$. Integrate the term $\psi\,\boldsymbol{U}\cdot\nabla\bar\rho$ by parts (see Remark 3.4.31) to obtain

$$\begin{aligned}\int_0^T\int_\Omega [\bar\rho_t\,\psi + \nabla\bar\rho\cdot\nabla\psi] + \int_0^T\int_\Gamma \bar\eta_t\,\psi + \int_0^T\int_{\Gamma^{\mathrm{out}}} \bar\rho\,\psi|\boldsymbol{U}_b\cdot\boldsymbol{\nu}| \\ = \int_0^T\int_\Omega [\psi\,\bar\rho\,\mathrm{div}\,\boldsymbol{U} + \bar\rho\,\boldsymbol{U}\cdot\nabla\psi]\,.\end{aligned} \tag{3.144}$$

For $M\subset\mathbb{R}$ denote the characteristic function of M by χ_M. In (3.144), choose $\psi = q_m$, where $q_m(\boldsymbol{x},\tau) = H_e^m(\bar\rho(\boldsymbol{x},\tau))\cdot\chi_{[0,t]}(\tau)$, $t\in(0,T]$ and

$$H_e^m(s) := \begin{cases} 0, & \text{if } s<0,\\ m\,s, & \text{if } 0\le s\le 1/m,\\ 1, & \text{if } s>1/m.\end{cases}$$

Note that $H_e^m(s) = 1-(m\,s^+-1)^-$ so that $H_e^m(\bar\rho)$ is an admissible testfunction due to Lemma 3.E.6.

The terms in (3.144) are estimated separately. The second summand under the first integral on the left-hand side can be estimated from below as follows

$$\int_\Omega \nabla\bar\rho\cdot\nabla q_m\,\mathrm{d}\boldsymbol{x} = \int_\Omega (H_e^m)'(\bar\rho)\,|\nabla\bar\rho|^2\,\mathrm{d}\boldsymbol{x} \ge 0. \tag{3.145}$$

The integral over Γ^{out} in (3.144) is positive due to (3.83). To estimate the term containing the divergence, use the relation $H_e^m(\bar\rho)\cdot\bar\rho\le\bar\rho^+$ and the assumptions on $\mathrm{div}\,\boldsymbol{U}$ to obtain the estimate

$$\left|\int_0^t\int_\Omega \bar\rho\cdot H_e^m(\bar\rho)\cdot\mathrm{div}\,\boldsymbol{U}\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau\right| \le C_U^*\int_0^t\int_\Omega \bar\rho^+\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau. \tag{3.146}$$

To estimate the last term on the right-hand side of (3.144) define

$$M_m := \left\{(\boldsymbol{x},\tau)\in\Omega\times(0,t)\;:\;0\le\bar\rho(\boldsymbol{x},\tau)\le m^{-1}\right\},$$

then, $\nabla H_e^m(\bar\rho) = \mathbf{0}$ in $\left[\Omega\times(0,T)\right]\setminus M_m$. Using Young's inequality yields the estimate

$$\begin{aligned}\left|\int_0^t\int_\Omega \bar\rho\,\boldsymbol{U}\cdot\nabla H_e^m(\bar\rho)\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau\right| &= \left|\int_{M_m}\bar\rho\,\boldsymbol{U}\cdot(H_e^m)'(\bar\rho)\cdot\nabla\bar\rho\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau\right|\\ &\le \frac{C_U^2}{2}\int_{M_m}\bar\rho^+\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau + \frac{1}{2}\int_{M_m}(H_e^m)'(\bar\rho)\,|\nabla\bar\rho|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau,\end{aligned} \tag{3.147}$$

because $0\le\bar\rho(\boldsymbol{x},t)\le m^{-1}$ on M_m so that $\bar\rho(\boldsymbol{x},t)\cdot(H_e^m)'(\bar\rho(\boldsymbol{x},t))\le 1$.

Substituting (3.145), (3.146), and (3.147) into (3.144) yields the inequality

$$\begin{aligned}\int_0^t\left[\int_\Omega \bar\rho_t\,H_e^m(\bar\rho)\,\mathrm{d}\boldsymbol{x} + \int_\Gamma \bar\eta_t\,H_e^m(\bar\rho)\,\mathrm{d}s\right]\mathrm{d}\tau + \frac{1}{2}\int_0^t\int_\Omega (H_e^m)'(\bar\rho)\,|\nabla\bar\rho|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau\\ \le C\int_0^t\int_\Omega \bar\rho^+\,\mathrm{d}\boldsymbol{x}\mathrm{d}\tau\end{aligned}$$

for $C = C_U^2/2 + C_U^*$. The passage to the limit as $m \to \infty$ yields:

$$\int_0^t \left[\int_\Omega \bar{\rho}_t \, q \, \mathrm{d}\boldsymbol{x} + \int_\Gamma \bar{\eta}_t \, q \, \mathrm{d}s \right] \mathrm{d}\tau \leq C \int_0^t \int_\Omega \bar{\rho}^+ \, \mathrm{d}\boldsymbol{x} \mathrm{d}\tau, \qquad (3.148)$$

where $q \in H_e(\bar{\rho})$ is a function such that $H_e^m(\bar{\rho}) \to q$ a.e. in $\Omega \times (0, T)$ and a.e in $\Gamma \times (0, T)$.

By (3.127), it holds $\bar{\eta} \in L^2(\Gamma; H^1(0, T))$. Thus, the second term on the left-hand side of (3.148) can be estimated from below using Theorem 3.C.1. It holds

$$\frac{\partial \, \bar{\eta}^+(\boldsymbol{x}, t)}{\partial t} \leq \frac{\partial \, \bar{\eta}(\boldsymbol{x}, t)}{\partial t} q(\boldsymbol{x}, t), \qquad \text{a. e. in } (0, T) \qquad (3.149)$$

for almost all $\boldsymbol{x} \in \Gamma$. Since $\bar{\rho}^0 = 0$ and $\bar{\eta}^0 = 0$, substituting (3.149) into (3.148) yields

$$\int_\Omega \bar{\rho}^+(t) \, \mathrm{d}\boldsymbol{x} + \int_\Gamma \bar{\eta}^+(t) \, \mathrm{d}s \leq C \int_0^t \int_\Omega \bar{\rho}^+ \, \mathrm{d}\boldsymbol{x} \mathrm{d}\tau.$$

Due to (3.173), it holds $\bar{\rho}^+ = 0$ and $\bar{\eta}^+ = 0$. By interchanging the indices 1 and 2, we conclude that $\bar{\rho} = 0$ and $\bar{\eta} = 0$. ☐

To complete the proof of Theorem 3.4.21, it remains to prove the embedding used in Section 3.4.2.4 to obtain the regularity given in (3.140).

3.4.2.6 An anisotropic embedding

This section is devoted to the anisotropic embedding theorem used in Section 3.4.2.4 to establish the relation (3.85). The embedding (see Theorem 3.4.34) and the method of proof presented here were communicated to me by Pavel Krejčí.

Throughout this section, assume that x^*, y^*, z^*, $t^* > 0$ are given, set $X := (0, x^*)$ and $X' := (-x^*, 2x^*)$, and define the intervals Y, Z, T, Y', Z', and T' analogously. Introduce the following notation:

$$\begin{aligned}
Q &= X \times Y \times Z \times T, \\
Q' &= X' \times Y' \times Z' \times T', \\
\boldsymbol{x} &= (x, y, z, t) = (x_1, x_2, x_3, x_4), \\
\boldsymbol{\lambda} &= (\lambda_1, \lambda_2, \lambda_3, \lambda_4), \\
|\boldsymbol{\lambda}| &= \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4, \\
\boldsymbol{x} : \sigma^{\boldsymbol{\lambda}} &= \left(\frac{x_1}{\sigma^{\lambda_1}}, \frac{x_2}{\sigma^{\lambda_2}}, \frac{x_3}{\sigma^{\lambda_3}}, \frac{x_4}{\sigma^{\lambda_4}} \right), \qquad \sigma > 0, \\
\|f(x, y, \cdot, \cdot)\|_{p, Z \times T} &= \left[\int_{Z \times T} |f(x, y, z, t)|^p \, \mathrm{d}z \, \mathrm{d}t \right]^{1/p},
\end{aligned}$$

with obvious changes if $p = \infty$. The following definition introduces the considered function spaces.

Definition 3.4.33. *For $p \geq 1$ define the following function spaces:*

$$V := V^p(Q) := \left\{u \in L^1(Q) \;:\; u_t \in L^2(Q),\; D_i u \in L^p(Q),\; i = 1, 2, 3\right\},$$
$$W := W^p(Q) := L^p\left(X \times Y\,;\, \mathcal{C}(\overline{Z \times T})\right),$$

endowed with the norms

$$\|u\|_{V^p(Q)} = \|u\|_{1,\,Q} + \|u_t\|_{2,\,Q} + \sum_{i=1}^{3} \|D_i u\|_{p,\,Q}\,,$$
$$\|u\|_{W^p(Q)} = \Big\| \|u(x, y, z, t)\|_{\infty,\,Z\times T} \Big\|_{p,\,X\times Y}\,.$$

The norms in $V^p(\mathbb{R}^4)$ and $W^p(\mathbb{R}^4)$ will simply be denoted by $\|\cdot\|_{V^p}$ and $\|\cdot\|_{W^p}$, respectively. The proof Theorem 3.4.34 is based on a prolongation operator $E_p : V^p(Q) \to V^p(\mathbb{R}^4)$ that is continuous in the norm given by Definition 3.4.33. To construct E_p, fix a ball $B \subset \mathbb{R}^4$ such that $\overline{Q} \subset B$, and define V_B^p to be the subset of $V^p(\mathbb{R}^4)$ consisting of all functions vanishing outside of B. Define W_B^p analogously. The operator E_p can be constructed similar to [9, Chapter 2, §3.6]. For a given $u \in V^p(Q)$, define the prolongation u_1 of u onto the set $X' \times Y \times Z \times T$ by reflection at the hyperplanes $\{x = 0\}$ and $\{x = x^*\}$. We obtain

$$u_1(x, y, z, t) := \begin{cases} u(x, y, z, t) & \text{if } x \in X, \\ u(-x, y, z, t) & \text{if } x \in (-x^*,\, 0), \\ u(x^* - (x - x^*), y, z, t) & \text{if } x \in (x^*,\, 2x^*). \end{cases}$$

In the same way, the function u_2 can be defined as the extension of u_1 onto $X' \times Y' \times Z \times T$. Proceeding in this way, yields a function $u_4 \in V^p(Q')$ with $\|u_4\|_{V^p(Q')} \leq 3^4\, \|u\|_{V^p(Q)}$. Fix a smooth cutoff function $\zeta \in \mathcal{D}(\mathbb{R}^4)$ satisfying $\zeta(\boldsymbol{x}) = 1$ if $\boldsymbol{x} \in Q$, and $\zeta(\boldsymbol{x}) = 0$ if $\boldsymbol{x} \notin B \cap Q'$. Define the operator E_p by $E_p\, u := \zeta \cdot u_4$. Then $E_p\, u \in V_B^p$ and, due to the choice of ζ, it holds:

$$\begin{aligned} \|E_p\, u\|_{1,\,\mathbb{R}^4} &\leq 3^4\, \|u\|_{1,\,Q}\,, \\ \|D_i(E_p\, u)\|_{p_i,\,\mathbb{R}^4} &\leq \|u_4\, D_i\zeta\|_{p_i,\,\mathbb{R}^4} + \|\zeta\, D_i u_4\|_{p_i,\,\mathbb{R}^4} \\ &\leq 3^4\, \|\zeta\|_{\mathcal{C}^1(\mathbb{R}^4)} \left(\|u\|_{p_i,\,Q} + \|D_i u\|_{p_i,\,Q}\right). \end{aligned} \tag{3.150}$$

Let us consider the case $p \in [2, 4]$. Since Q is bounded, Poincare's inequality (see for example [9, Chapter 1, Theorem 1.3]) yields

$$\|u\|_{2,\,Q} \leq C\Big(\|u\|_{1,\,Q} + \sum_i \|D_i u\|_{2,\,Q}\Big)$$

so that we obtain $u \in H^1(Q) \hookrightarrow L^4(Q),\; N = 4$. Thus, inequalities (3.150) yield

$$\|E_p\, u\|_{V^p} \leq c_p\, \|u\|_{V^p(Q)}\,, \qquad \text{for } p \in [2, 4]. \tag{3.151}$$

In the same way, a prolongation operator $E_p : W^p(Q) \to W_B^p$ can be defined.

The following theorem gives the result of this section.

Theorem 3.4.34. *Let $p \in (2,4]$. If q satisfies the following inequalities*

$$p \le q < \frac{4+2p}{6-p},$$

then the embedding $V^p(Q) \subset\subset W^q(Q)$ is compact.

The proof of Theorem 3.4.34 is divided into the following steps:

1. Definition of approximations u^σ.
2. Estimation of the difference $u^\alpha - u^\beta$ of approximations in the $W^q(Q)$-norm.
3. Proof of the continuity of the embedding $V^p(Q) \hookrightarrow W^q(Q)$.
4. Proof of the compactness of the embedding $V^q(Q) \subset\subset W^q(Q)$.

Implementation of Step 1: definition of approximations. For a given $u \in V^p(Q)$ denote the prolongation $E_p\, u$ by u_*. Define the approximations u^σ ($\sigma > 0$) of u as follows:

$$\begin{aligned} u^\sigma(\boldsymbol{x}) &= \sigma^{-|\boldsymbol{\lambda}|} \int_{\mathbb{R}^4} \phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) \cdot u_*(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' \\ &= \sigma^{-|\boldsymbol{\lambda}|} \int_{\mathbb{R}^4} \phi\left(\frac{x_1-x_1'}{\sigma^{\lambda_1}}\,,\ \frac{x_2-x_2'}{\sigma^{\lambda_2}}\,,\ \frac{x_3-x_3'}{\sigma^{\lambda_3}}\,,\ \frac{x_4-x_4'}{\sigma^{\lambda_4}}\right) \cdot u_*(\boldsymbol{x}')\, \mathrm{d}x_1' \dots \mathrm{d}x_4' \end{aligned} \tag{3.152}$$

where $\phi \in \mathcal{D}(\mathbb{R}^4)$ is a fixed positive smoothing function with $\int \phi\, \mathrm{d}\boldsymbol{x} = 1$. The derivative of u^σ with respect to σ is given by the following identity:

$$\begin{aligned} \frac{\partial u^\sigma}{\partial \sigma} &= -|\boldsymbol{\lambda}|\, \sigma^{-|\boldsymbol{\lambda}|-1} \int_{\mathbb{R}^4} \phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) \cdot u_*(\boldsymbol{x}')\, \mathrm{d}\boldsymbol{x}' \\ &\quad + \sigma^{-|\boldsymbol{\lambda}|} \int_{\mathbb{R}^4} \sum_i D_i\phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) (x_i - x_i')(-\lambda_i)\sigma^{-\lambda_i - 1} \cdot u_*(\boldsymbol{x}')\, \mathrm{d}\boldsymbol{x}' \\ &= \int_{\mathbb{R}^4} \sum_i (-\lambda_i)\, \sigma^{-|\boldsymbol{\lambda}|-1}\, u_*(\boldsymbol{x}') \cdot \left[\phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) + D_i\phi \cdot \frac{x_i - x_i'}{\sigma^{\lambda_i}}\right] \mathrm{d}\boldsymbol{x}'. \end{aligned} \tag{3.153}$$

Using the product rule, the following computation yields an expression for the terms in square brackets of (3.153):

$$\begin{aligned} &\frac{\partial}{\partial x_i'}\left[\frac{x_i - x_i'}{\sigma^{\lambda_i}} \cdot \phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right)\right] \\ &\quad = -\sigma^{-\lambda_i}\, \phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) + \frac{x_i - x_i'}{\sigma^{\lambda_i}} \cdot D_i\phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) \cdot \left(-\sigma^{-\lambda_i}\right) \\ &\quad = \frac{-1}{\sigma^{\lambda_i}} \cdot \left[\phi + \frac{x_i - x_i'}{\sigma^{\lambda_i}} \cdot D_i\phi\right]. \end{aligned}$$

Thus, the identity (3.153) can be rewritten as follows

$$\begin{aligned} \frac{\partial u^\sigma}{\partial \sigma} &= \sum_i \lambda_i\, \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i} \int_{\mathbb{R}^4} u_*(\boldsymbol{x}') \cdot \frac{-1}{\sigma^{\lambda_i}} \cdot \left[\phi + D_i\phi \cdot \frac{x_i - x_i'}{\sigma^{\lambda_i}}\right] \mathrm{d}\boldsymbol{x}' \\ &= \sum_i \lambda_i\, \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i} \int_{\mathbb{R}^4} u_*(\boldsymbol{x}') \cdot \frac{\partial}{\partial x_i'}\left[\frac{x_i - x_i'}{\sigma^{\lambda_i}} \cdot \phi\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right)\right] \mathrm{d}\boldsymbol{x}' \\ &= -\sum_i \lambda_i\, \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i} \int_{\mathbb{R}^4} \Phi_i\left((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\right) \cdot D_i\, u_*(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}', \end{aligned} \tag{3.154}$$

where $\Phi_i(\boldsymbol{y}) := y_i\,\phi(\boldsymbol{y})$.

Let u^α and u^β be two approximations, $0 < \alpha < \beta \le 1$. Using identity (3.154), we obtain the following estimate for the difference $u^\beta - u^\alpha$ of two approximations:

$$\left|u^\beta(\boldsymbol{x}) - u^\alpha(\boldsymbol{x})\right| \le \sum_{i=1}^{4} |\lambda_i|\ \mathcal{I}_i(\boldsymbol{x}), \tag{3.155}$$

where

$$\mathcal{I}_i(\boldsymbol{x}) = \int_\alpha^\beta \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i} \int_{\mathbb{R}^4} \left|\Phi_i\big((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\big)\right| \cdot \left|D_i\,u_*(\boldsymbol{x}')\right|\,\mathrm{d}\boldsymbol{x}'\,\mathrm{d}\sigma, \tag{3.156}$$

for $i = 1, \ldots, 4$.

Implementation of Step 2: estimate for the difference of approximations. To indicate the order of integration, we use the following notation:

$$\int_{\mathbb{R}_t} \mathrm{d}t = \int_{\mathbb{R}} \mathrm{d}t \qquad \text{or} \qquad \int_{\mathbb{R}_t} \mathrm{d}t' = \int_{\mathbb{R}} \mathrm{d}t'.$$

A similar notation is used when integrating over x, y, z, x', y', or z'. The following lemma gives estimates of the W^q-norm of the difference $u^\beta - u^\alpha$ in terms of the V^p-norm of a given $u \in V^p(Q)$ and certain $p, q \ge 1$.

Lemma 3.4.35. *Assume $\beta > \alpha > 0$ and $p \in (2, 4]$, and let q satisfy the inequalities*

$$p \le q < \frac{4+2p}{6-p}.$$

Then, the following estimate holds

$$\left\|u^\beta - u^\alpha\right\|_{W^q} \le C_{pq} \cdot (\beta^\kappa - \alpha^\kappa)\,\|u_*\|_{V^p}$$

for all $u \in V^p(Q)$, where

$$\kappa = \frac{1}{2} + \frac{p+2}{5p-6}\left(\frac{2}{q} - \frac{3}{2}\right) > 0,$$

$$C_{pq} = \frac{p+2}{5p-6} \sum_{i=1}^{3} \left\| \|\Phi_i\|_{p,\,\mathbb{R}_z\times\mathbb{R}_t} \right\|_{r,\,\mathbb{R}_x\times\mathbb{R}_y} + \left\| \|\Phi_4\|_{2,\,\mathbb{R}_z\times\mathbb{R}_t} \right\|_{s,\,\mathbb{R}_x\times\mathbb{R}_y},$$

and

$$\frac{1}{r} = 1 + \frac{1}{q} - \frac{1}{p}, \qquad \frac{1}{s} = \frac{1}{2} + \frac{1}{q}.$$

Proof. Estimate the W^q-norm of the integrals $\mathcal{I}_i$ appearing in (3.155). To this end, set $p_i = p$, $i = 1, 2, 3$, and $p_4 = 2$, and estimate the integrand in (3.156) in the following way. Apply

Hölder's inequality in the variables z' and t', and substitute $y_i = x_i/\sigma^{\lambda_i}$ to obtain

$$\begin{aligned}
&\sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i} \int_{\mathbb{R}^4} \left|\Phi_i\big((\boldsymbol{x}-\boldsymbol{x}') : \sigma^{\boldsymbol{\lambda}}\big)\right| \cdot \left|D_i\, u_*(\boldsymbol{x}')\right| \, \mathrm{d}\boldsymbol{x}' \\
&\quad \le \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i} \int_{\mathbb{R}_x} \int_{\mathbb{R}_y} \left\|\Phi_i\left(\frac{x-x'}{\sigma^{\lambda_1}},\, \frac{y-y'}{\sigma^{\lambda_2}},\, \frac{\cdot}{\sigma^{\lambda_3}},\, \frac{\cdot}{\sigma^{\lambda_4}}\right)\right\|_{p_i',\, \mathbb{R}_z\times\mathbb{R}_t} \\
&\qquad \times \left\|D_i\, u_*\left(x',\, y',\, \cdot,\, \cdot\right)\right\|_{p_i,\, \mathbb{R}_z\times\mathbb{R}_t} \, \mathrm{d}y'\, \mathrm{d}x' \\
&\quad = \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i+(\lambda_3/p_i')+(\lambda_4/p_i')} \int_{\mathbb{R}_x} \int_{\mathbb{R}_y} \left\|\Phi_i\left(\frac{x-x'}{\sigma^{\lambda_1}},\, \frac{y-y'}{\sigma^{\lambda_2}},\, \cdot,\, \cdot\right)\right\|_{p_i',\, \mathbb{R}_z\times\mathbb{R}_t} \\
&\qquad \times \left\|D_i\, u_*\left(x',\, y',\, \cdot,\, \cdot\right)\right\|_{p_i,\, \mathbb{R}_z\times\mathbb{R}_t} \, \mathrm{d}y'\, \mathrm{d}x'.
\end{aligned}$$

Therefore, the $\mathcal{C}(\overline{\mathbb{R}_z \times \mathbb{R}_t})$-norm of $\mathcal{I}_i(x, y, \cdot, \cdot)$ can be estimated as follows

$$\begin{aligned}
\|\mathcal{I}_i(x, y, \cdot, \cdot)\|_{\infty,\, \mathbb{R}_z\times\mathbb{R}_t} \le \int_\alpha^\beta \Bigg[&\sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i+(\lambda_3/p_i')+(\lambda_4/p_i')} \\
&\times \int_{\mathbb{R}_x} \int_{\mathbb{R}_y} \left\|\Phi_i\left(\frac{x-x'}{\sigma^{\lambda_1}},\, \frac{y-y'}{\sigma^{\lambda_2}},\, \cdot,\, \cdot\right)\right\|_{p_i',\, \mathbb{R}_z\times\mathbb{R}_t} \\
&\times \left\|D_i\, u_*\left(x',\, y',\, \cdot,\, \cdot\right)\right\|_{p_i,\, \mathbb{R}_z\times\mathbb{R}_t} \Bigg] \, \mathrm{d}y'\, \mathrm{d}x'\, \mathrm{d}\sigma
\end{aligned} \tag{3.157}$$

Due to Minkowski's inequality, we obtain the following estimate of the W^q-norm of $\mathcal{I}_i$:

$$\begin{aligned}
\|\mathcal{I}_i\|_{W^q} &= \left\| \|\mathcal{I}_i(\cdot, \cdot, \cdot, \cdot)\|_{\infty,\, \mathbb{R}_z\times\mathbb{R}_t} \right\|_{q,\, \mathbb{R}_x\times\mathbb{R}_y} \\
&\le \int_\alpha^\beta \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i+(\lambda_3/p_i')+(\lambda_4/p_i')} \\
&\quad \times \left\{ \int_{\mathbb{R}_x\times\mathbb{R}_y} \left[\int_{\mathbb{R}_x\times\mathbb{R}_y} \left\|\Phi_i\left(\frac{x-x'}{\sigma^{\lambda_1}},\, \frac{y-y'}{\sigma^{\lambda_2}},\, \cdot,\, \cdot\right)\right\|_{p_i',\, \mathbb{R}_z\times\mathbb{R}_t} \right.\right. \\
&\quad \left.\left. \times \left\|D_i\, u_*\left(x',\, y',\, \cdot,\, \cdot\right)\right\|_{p_i,\, \mathbb{R}_z\times\mathbb{R}_t} \, \mathrm{d}x'\, \mathrm{d}y' \right]^q \mathrm{d}x\, \mathrm{d}y \right\}^{1/q} \mathrm{d}\sigma.
\end{aligned} \tag{3.158}$$

Note that the curly braces represent the $L^q(\mathbb{R}_x \times \mathbb{R}_y)$-norm of a convolution. Apply Young's inequality for convolutions in (3.158) with

$$\frac{1}{p_i} + \frac{1}{r_i} = 1 + \frac{1}{q}, \tag{3.159}$$

to obtain the following estimate

$$\begin{aligned}
\|\mathcal{I}_i\|_{W^q} &\le \int_\alpha^\beta \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i+(\lambda_3/p_i')+(\lambda_4/p_i')} \\
&\quad \times \left\| \left\|\Phi_i\left(\frac{\cdot}{\sigma^{\lambda_1}},\, \frac{\cdot}{\sigma^{\lambda_2}},\, \cdot,\, \cdot\right)\right\|_{p_i',\, \mathbb{R}_z\times\mathbb{R}_t} \right\|_{r_i,\, \mathbb{R}_x\times\mathbb{R}_y} \cdot \|D_i\, u_*\|_{p_i,\, \mathbb{R}^4} \, \mathrm{d}\sigma \\
&\le c_p \int_\alpha^\beta \sigma^{-1-|\boldsymbol{\lambda}|+\lambda_i+(\lambda_3/p_i')+(\lambda_4/p_i')+(\lambda_1/r_i)+(\lambda_2/r_i)} \, \mathrm{d}\sigma \\
&\quad \times \left\| \|\Phi_i\|_{p_i',\, \mathbb{R}_z\times\mathbb{R}_t} \right\|_{r_i,\, \mathbb{R}_x\times\mathbb{R}_y} \cdot \|u\|_{V^p(Q)} \,.
\end{aligned} \tag{3.160}$$

Remember that $p_i = p$ $(i = 1, 2, 3)$ and $p_4 = 2$, so that $r_1 = r_2 = r_3 = r$ and $r_4 = s$, where r and s are defined in the lemma. The requirement $r, s \geq 1$ and the identity (3.159) yield the following lower bound for q:

$$q \geq \max\{p,\, 2\}. \tag{3.161}$$

The integral on the right-hand side of (3.160) remains bounded for arbitrary $\beta > \alpha > 0$, if the exponents of σ are greater than -1 for $i = 1, \ldots, 4$. Equalize the exponents for $i = 1, \ldots, 4$ to obtain

$$\begin{aligned} 0 < \kappa := \lambda_1 + \frac{\lambda_3}{p'} + \frac{\lambda_4}{p'} + \frac{\lambda_1}{r} + \frac{\lambda_2}{r} - |\boldsymbol{\lambda}| &= \lambda_2 + \frac{\lambda_3}{p'} + \frac{\lambda_4}{p'} + \frac{\lambda_1}{r} + \frac{\lambda_2}{r} - |\boldsymbol{\lambda}| \\ = \lambda_3 + \frac{\lambda_3}{p'} + \frac{\lambda_4}{p'} + \frac{\lambda_1}{r} + \frac{\lambda_2}{r} - |\boldsymbol{\lambda}| &= \lambda_4 + \frac{\lambda_3}{2} + \frac{\lambda_4}{2} + \frac{\lambda_1}{s} + \frac{\lambda_2}{s} - |\boldsymbol{\lambda}|. \end{aligned} \tag{3.162}$$

The first two equations in (3.162) imply the relations

$$\lambda_1 = \lambda_2 = \lambda_3 =: \lambda, \qquad \lambda_4 =: \mu, \qquad \text{and} \qquad |\boldsymbol{\lambda}| = 3\,\lambda + \mu.$$

Thus, the last equation in (3.162) yields

$$\lambda \left(\frac{1}{2} + \frac{1}{p'} + \frac{2}{r} - \frac{2}{s} \right) = \mu \left(\frac{3}{2} - \frac{1}{p'} \right). \tag{3.163}$$

Substituting $1/p' = 1 - 1/p$ and the identities for $1/r$ and $1/s$ given in the lemma into (3.163) yields

$$\lambda\,(5p - 6) = \mu\,(p + 2)\,.$$

Choosing $\mu = 1$ and using (3.162) yield the identities

$$\lambda = \frac{p + 2}{5p - 6} \qquad \text{and} \qquad \kappa = \frac{1}{2} + \lambda \left(\frac{2}{q} - \frac{3}{2} \right). \tag{3.164}$$

Moreover, the inequality of (3.162) holds, if q satisfies the inequality

$$q < \frac{2(p + 2)}{6 - p}. \tag{3.165}$$

Combining the lower and upper bounds of q given by (3.161) and (3.165), we obtain the following inequality for p:

$$p < \frac{2(p + 2)}{6 - p}, \qquad \text{which holds for} \qquad p \in (2,\, 6). \tag{3.166}$$

Due to (3.162), the integral on the right-hand side of (3.160) satisfies the relations

$$0 < \int_{\alpha}^{\beta} \sigma^{\kappa - 1}\, \mathrm{d}\sigma = \beta^{\kappa} - \alpha^{\kappa} < \beta^{\kappa}, \qquad \text{for} \quad \beta > \alpha > 0. \tag{3.167}$$

The lemma follows from (3.161), (3.164), (3.165), (3.166) and (3.167). □

Implementation of Step 3: continuity of the embedding. The next lemma ensures that $W^q(Q) \subset V^p(Q)$ with continuous injection if p and q satisfy the requirements of Lemma 3.4.35.

Lemma 3.4.36. *Let* $p \in (2, 4]$. *If* q *satisfies the inequalities*

$$p \le q < \frac{4+2p}{6-p},$$

then the embedding $W^q(Q) \hookrightarrow V^p(Q)$ *is continuous. The following estimate*

$$\|u_*\|_{W^q} \le C_q\, \sigma^\delta\, \|u_*\|_{1,\mathbb{R}^4} + \sigma^\kappa\, \|u_*\|_{V^p}$$

holds for all $u \in V^p(Q)$ *and* $\sigma > 0$*, where*

$$C_q = \Big\| \|\phi\|_{\infty,\mathbb{R}_z\times\mathbb{R}_t} \Big\|_{q,\mathbb{R}_x\times\mathbb{R}_y}, \qquad \delta = -|\boldsymbol{\lambda}| + \frac{2\lambda}{q},$$

λ *and* κ *are defined by* (3.164)*, and* $\boldsymbol{\lambda} = (\lambda, \lambda, \lambda, 1)$.

Proof. In the definition (3.152) of u^σ, apply Hölder's inequality in the varialbles z' and t' to obtain the estimate

$$\|u^\sigma(x,y,\cdot,\cdot)\|_{\infty,\mathbb{R}_z\times\mathbb{R}_t} \le \sigma^{-|\boldsymbol{\lambda}|} \int_{\mathbb{R}_x\times\mathbb{R}_y} \left\| \phi\left(\frac{x-x'}{\sigma^\lambda},\, \frac{y-y'}{\sigma^\lambda},\, \cdot,\, \cdot\right)\right\|_{\infty,\mathbb{R}_z\times\mathbb{R}_t}$$
$$\times \left\|u_*\left(x',\, y',\, \cdot,\, \cdot\right)\right\|_{1,\mathbb{R}_z\times\mathbb{R}_t} \,\mathrm{d}x'\,\mathrm{d}y'.$$

Computing the $L^q(\mathbb{R}_x \times \mathbb{R}_y)$-norm of both sides and applying Young's inequality for convolutions yield

$$\|u^\sigma\|_{W^q} \le \sigma^\delta \cdot \Big\| \|\phi\|_{\infty,\mathbb{R}_z\times\mathbb{R}_t} \Big\|_{q,\mathbb{R}_x\times\mathbb{R}_y} \cdot \Big\| \|u_*\|_{1,\mathbb{R}_z\times\mathbb{R}_t} \Big\|_{1,\mathbb{R}_x\times\mathbb{R}_y}, \tag{3.168}$$

where $\delta = -|\boldsymbol{\lambda}| + \frac{2\lambda}{q}$. Applying the triangle inequality, inequality (3.168), and Lemma 3.4.35 we obtain the estimate

$$\|u\|_{W^q(Q)} \le \|u_*\|_{W^q} \le \|u^\sigma\|_{W^q} + \|u^\sigma - u_*\|_{W^q} \le C_q\, \sigma^\delta\, \|u_*\|_{1,\mathbb{R}^4} + C_{pq}\, \sigma^\kappa\, \|u_*\|_{V^p},$$

for $\sigma > 0$. □

Implementation of Step 4: compactness of the embedding. The proof of Theorem 3.4.34 is complete, if we show that every bounded subset $M \subset V^p(Q)$ is precompact in $W^q(Q)$, that is,

$$\forall \epsilon > 0 \;\; \exists u_1, \ldots, u_n \;\; \forall u \in M \;\; \exists k \in \{1, \cdots, n\} \;:\; \|u - u_k\|_{W^q(Q)} < \epsilon.$$

To this end, let $\epsilon > 0$, p and q satisfy the requirements of Lemma 3.4.36, and M be a bounded subset of $V^p(Q)$. Fix $\sigma \in (0,1)$ such that the following inequality holds:

$$\|u_* - u^\sigma\|_{W^q} \le C_{pq}\, \sigma^\kappa\, \|u_*\|_{V^p} < \frac{\epsilon}{4} \qquad \forall u \in M, \tag{3.169}$$

where the constants C_{pq} and κ are defined by Lemma 3.4.35.

Set $M_\sigma := \{u^\sigma \ : \ u \in M\}$ and remember that $u_* = E_p\, u \in V_B^p$ by the construction of the prolongation operator E_p. Thus, the definition (3.152) of u^σ implies the relation $\operatorname{supp} u^\sigma \subset B_\phi$, where $B_\phi := B + \operatorname{supp}\phi$.

The set M_σ is bounded in $\mathcal{C}^1(\overline{B_\phi})$ and therefore pre-compact in $\mathcal{C}^0(\overline{B_\phi})$ by the Theorem of Arzela-Ascoli. Thus, there exist $u_1, \ldots, u_n \in M$ such that

$$\forall u \in M \ \ \exists k \in \{1, \ldots, n\} \ \ \forall \boldsymbol{x} \in B_\phi \ : \ \|u^\sigma - u_k^\sigma\|_{\infty,\, B_\phi} < \frac{\epsilon}{4\ |P_{x,y}\, B_\phi|^{1/q}}, \tag{3.170}$$

where $|P_{x,y}\, B_\phi|$ is the two dimensional measure of the projection of B_ϕ onto the x, y-plane. Let $u \in M$. Due to inequality (3.169) and property (3.170), there exists $k \in \{1, \ldots, n\}$ such that

$$\|u_* - u_k^\sigma\|_{W^q} \le \|u_* - u^\sigma\|_{W^q} + \|u^\sigma - u_k^\sigma\|_{W^q} < \frac{\epsilon}{2}. \tag{3.171}$$

Set $M_k = \{u \in M : \|u_* - u_k^\sigma\|_{W^q} < \epsilon/2\}$, $k = 1, \ldots, n$, and $J = \{k \in \{1, \ldots, n\} : M_k \neq \emptyset\}$. For every $k \in J$ fix one representative $\hat{u}_k \in M_k$. Due to (3.171), the following estimates

$$\|u - \hat{u}_k\|_{W^q(Q)} \le \|u_* - \hat{u}_{k,*}\|_{W^q} \le \|u_* - u_k^\sigma\|_{W^q} + \|u_k^\sigma - \hat{u}_{k,*}\|_{W^q} < \epsilon$$

hold for every $u \in M_k$. Moreover, we have $M = \bigcup_{k \in J} M_k$ by (3.170) and (3.171). The proof of Theorem 3.4.34 is complete.

This finishes the proof of Theorem 3.4.21 and the consideration of the evolution of the particle density. The consequences of Theorems 3.4.4 and 3.4.21 for the decoupled measurement problem are given in Theorem 3.4.1. Results from the literature are given in the appendix.

3.A Elementary inequalities

Theorem 3.A.1 (Young's inequality, see [47, Formula 1.1.4]). *Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^N$, $p > 1$ and $p^{-1} + q^{-1} = 1$, then*

$$\sum_{j=1}^{N} |x_j\, y_j| \leq \frac{1}{p} \sum_{j=1}^{N} \epsilon^p |x_j|^p + \frac{1}{q} \sum_{j=1}^{N} \epsilon^{-q} |y_j|^p.$$

Theorem 3.A.2 (Hölder's inequaltity). *Let $1 \leq p \leq \infty$ and $p^{-1} + q^{-1} = 1$ (with the convention $\infty^{-1} = 0$). Let $(\Omega,\, \Sigma,\, \mu)$ be a measurespace, $f \in L^p(\Omega)$, and $g \in L^q(\Omega)$. Then $f \cdot g \in L^1(\Omega)$ and*

$$\int_\Omega |f\, g| \,\mathrm{d}\mu \leq \left[\int_\Omega |f|^p \,\mathrm{d}\mu\right]^{1/p} \left[\int_\Omega |g|^q \,\mathrm{d}\mu\right]^{1/q}.$$

Proof. See [65, Theorem I.1.10] □

Theorem 3.A.3 (Minkowski's inequaltity). *Assume $1 < p < \infty$ and let $(\Omega,\, \Sigma,\, \mu)$ be measure space, and f and g be measurable functions on Ω with range in $[0, \infty]$. Then*

$$\left[\int_\Omega (f+g)^p \,\mathrm{d}\mu\right]^{1/p} \leq \left[\int_\Omega f^p \,\mathrm{d}\mu\right]^{1/p} + \left[\int_\Omega g^p \,\mathrm{d}\mu\right]^{1/p}.$$

Proof. See [51, Theorem 3.5] or [27, 198]. □

Theorem 3.A.4 (Generalized Minkowski's inequality). *In analogy to Theorem 3.A.3, it holds for $1 < p < \infty$:*

$$\left\{\int \left[\int |f(\boldsymbol{x}, \boldsymbol{y})| \,\mathrm{d}\lambda(\boldsymbol{y})\right]^p \mathrm{d}\mu(\boldsymbol{x})\right\}^{1/p} \leq \int \left[\int |f(\boldsymbol{x}, \boldsymbol{y})|^p \,\mathrm{d}\lambda(\boldsymbol{y})\right]^{1/p} \mathrm{d}\mu(\boldsymbol{x})$$

Proof. See [27, 202] or [51, Chapter 8, Excercise 16]. □

Lemma 3.A.5 (See [8]). *Let $f : \mathbb{R} \to \mathbb{R}$ be a C^1 function such that f' does not decrease. Then*

$$f(\alpha) - f(\beta) \leq f'(\alpha)(\alpha - \beta) \qquad \text{for all } \alpha, \beta \in \mathbb{R}.$$

3.B Gronwall type inequalities

Lemma 3.B.1 ([18, 8.2.29 Lemma]). *Let us assume that h is continuous, r is integrable in $[a, b]$, $h, r \geq 0$ in $[a, b]$, and that y is continuous in $[a, b]$ and satisfies the inequality*

$$y(t) \leq h(t) + \int_a^t r(s)\, y(s) \,\mathrm{d}s \qquad \forall t \in [a, b].$$

Then

$$y(t) \leq h(t) + \int_a^t r(s)\, h(s)\, \exp\left(\int_s^t r(\tau) \,\mathrm{d}\tau\right) \mathrm{d}s, \qquad t \in [a, b].$$

Lemma 3.B.1 will mainly be used in one of the following forms. By direct computation one verifies

$$y(t) \le \|h\|_{L^\infty(a,b)} \cdot \exp\left(\|r\|_{L^1(a,b)}\right). \tag{3.172}$$

Assume now that z is a non-negative real-valued function on $[a,b]$, and the inequality

$$y(t) + z(t) \le h(t) + \int_a^t r(s)\, y(s)\,\mathrm{d}s$$

holds for all $t \in [a,b]$. Then, y satisfies 3.172, and we obtain the following inequality

$$y(t) + z(t) \le \|h\|_{L^\infty(a,b)} \left[1 + \|r\|_{L^1(a,b)} \exp\left(\|r\|_{L^1(a,b)}\right)\right]. \tag{3.173}$$

The next lemma and the method of proof were communicated to me by Pavel Krejčí. For different Gronwall type inequalities, we refer to papers [48, 49].

Lemma 3.B.2. *Let f and u be real-valued nonnegative functions defined for $t \ge 0$ and let $p > 1$ be a constant. Assume $f \in L^1_{loc}(0,\infty)$, $u \in L^\infty_{loc}(0,\infty)$, and that the inequality*

$$u^p(t) \le C + \int_0^t f(s)\, u(s)\,\mathrm{d}s$$

holds true for all $t \ge 0$, where $C \ge 0$ is a constant. Then

$$u(t) \le \left[C^{(p-1)/p} + \frac{p-1}{p} \int_0^t f(s)\,\mathrm{d}s\right]^{1/(p-1)}$$

for all $t \ge 0$.

Proof. Define the function

$$g(t) := \left(C + \int_0^t f(s)\, u(s)\,\mathrm{d}s\right)^{1/p}.$$

Then g is absolutely continuous, $g(t) \ge u(t)$, and it holds

$$\frac{\mathrm{d}\, g^p}{\mathrm{d}t}(t) = p\, g^{p-1}(t)\, \dot g(t) = f(t)\, u(t) \le f(t)\, g(t).$$

Since $p - 2 > -1$, we obtain

$$\frac{p}{p-1}\, g^{p-1}(t) \le \frac{p}{p-1}\, g^{p-1}(0) + \int_0^t f(s)\,\mathrm{d}s.$$

This inequality and the relation $u(t) \le g(t),\ t \ge 0$, prove the lemma. □

We derive an inequality similar to (3.173). Assume u satisfies

$$u^2(t) + z(t) \le c^2 + 2 \int_0^t f(s) u(s)\,\mathrm{d}s$$

for a nonnegative function z. Then, Lemma 3.B.2 yields

$$\begin{aligned} u^2(t) + z(t) &\le c^2 + 2\,c \int_0^t f(s)\, ds + 2 \left(\int_0^t f(s)\, ds\right)^2 \\ &\le c^2 + 2\,c\,T^{1/2}\, \|f\|_{L^2(0,T)} + 2\,T\, \|f\|^2_{L^2(0,T)} \\ &\le 2\,c^2 + 3\,T\, \|f\|^2_{L^2(0,T)}, \end{aligned} \tag{3.174}$$

provided that f is square integrable over $(0,T)$ for $T \ge t$.

3.C Hilpert's inequality

The contents of this section is taken from [63, III.2]. Denote by H_e the Heaviside graph:

$$H_e(s) := \begin{cases} \{0\} & \text{if } s < 0, \\ [0,1] & \text{if } s = 0, \\ \{1\} & \text{if } s > 0, \end{cases}$$

and introduce generalized plays as follows. Assume that two functions γ_l and γ_r are given with

$$\gamma_l,\, \gamma_r : \mathbb{R} \to [-\infty, \infty] \qquad \text{continuous and nondecreasing, with} \qquad \gamma_r \leq \gamma_l. \tag{3.175}$$

For $\sigma \in \mathbb{R}$ set $J(\sigma) = [\gamma_r(\sigma),\, \gamma_l(\sigma)]$, and denote by $I_{J(\sigma)}$ the indicator function of $J(\sigma)$. The generalized play corresponds to the inclusion

$$\dot{\epsilon} \in -\partial I_{J(\sigma)}(\epsilon),$$

which is equivalent to the variational inequality

$$\epsilon \in J(\sigma), \qquad \dot{\epsilon}(\epsilon - v) \leq 0, \qquad \forall v \in J(\sigma).$$

For generalized plays the relation $\sigma \mapsto \epsilon$ can be expressed in the form

$$\epsilon(t) = [\mathcal{E}(\sigma,\, \epsilon^0)](t) \qquad \text{in } [0, T], \tag{3.176}$$

where $\mathcal{E}$ is a hysteresis operator. In (3.176) σ denotes a function $\tau \mapsto \sigma(\tau)$.

Hilpert's inequality is formulated in the following theorem.

Theorem 3.C.1 ([63, Theorem III.2.6]). *Let $(\sigma_i, \epsilon^0) \in W^{1,1}(0,T) \times \mathbb{R}$ $(i = 1, 2)$, and $h : [0,T] \to \mathbb{R}$ be a measurable function such that $h \in H_e(\sigma_1 - \sigma_2)$ a.e. in $(0,T)$. Set $\epsilon_i := \mathcal{E}(\sigma_i, \epsilon^0)$, $\bar{\epsilon} := \epsilon_1 - \epsilon_2$. Then*

$$\frac{\mathrm{d}\bar{\epsilon}}{\mathrm{d}t} h \geq \frac{\mathrm{d}}{\mathrm{d}t}(\bar{\epsilon}^+) \qquad \text{a.e. in } (0,T).$$

3.D Convergence theorems

Definition 3.D.1 (Weak convergence.). *Let X be a Banach space, and denote its dual by X'.*

1. *A sequence $\{x_k\}_{k\in\mathbb{N}}$ converges weakly to $x \in X$ as $k \to \infty$ ($x_k \rightharpoonup x$) if*

$$\langle x_k\,;\, x' \rangle \to \langle x\,;\, x' \rangle \qquad \text{for all } x' \in X'.$$

2. *A sequence $\{x'_k\}_{k\in\mathbb{N}}$ converges weakly to $x' \in X'$ as $k \to \infty$ ($x'_k \overset{*}{\rightharpoonup} x'$) if*

$$\langle x\,;\, x'_k \rangle \to \langle x\,;\, x' \rangle \qquad \text{for all } x \in X.$$

3. *A set $M \subset X$ (resp. X') is weakly (resp. $*$-weakly) sequentially compact if every sequence in M has a weakly (resp. $*$-weakly) convergent subsequence whose weak (resp. $*$-weak) limit lies in M.*

Remark 3.D.2 ([2, 6.3]). *1. The weak (resp. $*$-weak) limit of a sequence is unique.*

2. *Strong convergence implies weak or $*$-weak convergence.*
3. $x'_k \overset{*}{\rightharpoonup} x'$ *in* X' *implies* $\|x'\| \leq \liminf_{k\to\infty} \|x'_k\|$.
4. $x_k \rightharpoonup x$ *in* X *implies* $\|x\| \leq \liminf_{k\to\infty} \|x_k\|$.
5. *Weakly ($*$-weakly) convergent subsequences are bounded.*
6. *If* $x_k \to x$ *(strongly) in* X *and* $x'_k \overset{*}{\rightharpoonup} x'$ *in* X'*, then* $\langle x_k\,;\,x'_k\rangle \to \langle x\,;\,x'\rangle$*. The same holds true if* $x_k \rightharpoonup x$ *in* X *and* $x'_k \to x'$ *(strongly) in* X'.

Theorem 3.D.3 (Sequencial compactness, see [2, 6.5, 6.9])**.**

1. *Let* X *be separable. Then the close unit ball* $\overline{B_1(0)}$ *in* X' *is $*$-weakly sequentially compact.*
2. *Let* X *be reflexive. Then the close unit ball* $\overline{B_1(0)}$ *in* X *is weakly sequentially compact.*

3.E Sobolev spaces

For a nonnegative integer k and $1 \leq p \leq \infty$ define the Sobolev space $W^{k,p}(\Omega)$ by

$$W^{k,p}(\Omega) = \{u \in L^p(\Omega) \ : \ D^\alpha u \in L^p(\Omega) \text{ for all multiindices } 0 \leq |\alpha| \leq k\}\,.$$

Equipped with the norm

$$\|u\|_{W^{k,p}(\Omega)} = \Big(\sum_{0\leq|\alpha|\leq k} \|D^\alpha u\|^p_{L^p(\Omega)} \Big)^{1/p},$$

the space $W^{k,p}(\Omega)$ is a Banach-space ([1, 3.2 Theorem], [16, Section 5.2, Theorem 2]) and can be characterised as the completion of $\{u \in \mathcal{C}^k(\Omega) \ : \ \|u\|_{W^{k,p}(\Omega)} < \infty\}$ with respect to the norm $\|\cdot\|_{W^{k,p}(\Omega)}$ ([1, 3.16 Theorem], [2, 2.23 Theorem], [16, Section 5.3, Theorem 2]). For $\epsilon \in (0,1)$ set

$$I_{\alpha,\epsilon,p}(u) = \int_\Omega \int_\Omega \frac{|D^\alpha u(\boldsymbol{x}) - D^\alpha u(\boldsymbol{y})|^p}{|\boldsymbol{x}-\boldsymbol{y}|^{N+p\epsilon}} \,\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}.$$

The Sobolev-Slobodetskii space $W^{k+\epsilon,p}(\Omega)$ denotes the space of all functions $u \in W^{k,p}(\Omega)$ having finite norm

$$\|u\|_{W^{k+\epsilon,p}(\Omega)} = \Big[\|u\|^p_{W^{k,p}(\Omega)} + \sum_{|\alpha|=k} I_{\alpha,\epsilon,p}(u) \Big]^{1/p}.$$

As usual, $W^{l,p}_0(\Omega)$ denotes the closure of $\mathcal{C}^\infty_0(\Omega)$ in $W^{l,p}(\Omega)$, and $W^{-l,p}(\Omega) = \big(W^{l,p}_0(\Omega)\big)'$. The spaces $W^{l,2}(\Omega)$ are Hilbert spaces, and we use the following notation $H^l(\Omega) = W^{l,2}(\Omega)$ and $H^l_0(\Omega) = W^{l,2}_0(\Omega)$.

Some properties of Sobolev spaces depend on the smoothness of the boundary of Ω. Similar to [66, Defintion 2.7], define the smoothness of a domain as follows.

Definition 3.E.1 ((k,κ)-smooth domains)**.** *A domain $\Omega \subset \mathbb{R}^N$ is called (k,κ)-smooth if for each $\boldsymbol{x} \in \partial\Omega$ there exists a neighbourhood U_x such that*

1. *U_x is (k,κ)-diffeomorph to the unit cube $W^N = \{\boldsymbol{x} : |x_i| \le 1,\, i = 1,...,N\}$. Denote the 1-1-transformation $U_x \leftrightarrow W^N$ by Φ_x. The transformation Φ_x is supposed to have the following properties:*
2. *$U_x \cap \partial\Omega \leftrightarrow W^N \cap \{x_N = 0\}$.*
3. *$U_x \cap \Omega \leftrightarrow W^N \cap \{0 < x_N < 1\}$.*
4. *$U_x \cap (\mathbb{R}^N \setminus \overline{\Omega}) \leftrightarrow W^N \cap \{-1 < x_N < 0\}$.*

If Ω is $(0,1)$-smooth we say, Ω has Lipschitz boundary, or Ω is a Lipschitz domain. Denote by γ the operator defined by $(\gamma\, u) = u|_{\partial\Omega}$ when u is a smooth function. The next theorem considers the trace operator in Sobolev spaces $H^l(\Omega)$.

Theorem 3.E.2 (Trace Theorem, see [66, Theorems 8.7, 8.8])**.** *Let Ω be (k,κ)-smooth and assume that $1/2 < l \le k + \kappa$, (if l is integral, then $k = l - 1$, $\kappa = 1$ is admissible).*

1. *There exists a linear continuous operator*
$$S_0 : H^l(\Omega) \to H^{l-1/2}(\partial\Omega),$$
such that
$$S_0\phi = \phi|_{\partial\Omega}$$
for all $\phi \in \mathcal{C}^l(\overline{\Omega})$ for l integral, $\phi \in \mathcal{C}^{[l]+1}(\overline{\Omega})$ otherwise.
2. *There exists a linear continuous extension operator*
$$L_0 : H^{l-1/2}(\partial\Omega) \to H^l(\Omega)$$
such that
$$S_0(L_0(\phi)) = \phi \qquad \text{for all } \phi \in H^{l-1/2}(\partial\Omega).$$

The trace operator in Sobolev spaces $W^{s,p}(\Omega)$, $p > 1$, is considered, for example, in [25]. See also [9] for the case where s is positive integer, and [22] for the case $s = 1$.

Theorem 3.E.3 ([25, Theorem 1.5.1.3])**.** *Let Ω be a bounded open subset of $\mathbb{R}^N$ with a $\mathcal{C}^{k,1}$ boundary $\partial\Omega$. Assume that $s - 1/p$ is not an integer, $s \le k+1$, $s - 1/p = l + \sigma$, $0 < \sigma < 1$, l a non-negative integer. Then the mapping*
$$u \mapsto \left\{\gamma\, u,\ \gamma\frac{\partial u}{\partial \boldsymbol{\nu}},\ \dots,\ \gamma\frac{\partial^l u}{\partial \boldsymbol{\nu}^l}\right\}$$
which is defined for $u \in \mathcal{C}^{k,1}(\overline{\Omega})$, has a unique continuous extension as an operator from
$$W^{s,p}(\Omega) \quad \text{onto} \quad \prod_{j=0}^{l} W^{s-j-1/p,\,p}(\partial\Omega).$$
This operator has a right continuous inverse which does not depend on p.

Theorem 3.E.4 (Weak Gaussian Theorem [2, A 6.8])**.** *Let* $1 \le p \le \infty$, $p' = p/(p-1)$ *and* Ω *be a bounded Lipschitz domain.*

1. *If* $u \in W^{1,1}(\Omega)$*, then it holds for* $i = 1, ..., N$

$$\int_\Omega \frac{\partial u}{\partial x_i}\, \mathrm{d}\boldsymbol{x} = \int_{\partial\Omega} u \cdot \nu_i \, ds$$

2. *If* $u \in W^{1,p}(\Omega)$, $v \in W^{1,p'}(\Omega)$*, then Green's formula*

$$\int_\Omega \left[u \frac{\partial v}{\partial x_i} + v \frac{\partial u}{\partial x_i} \right] \mathrm{d}\boldsymbol{x} = \int_{\partial\Omega} S(u) \cdot S(v) \cdot \nu_i \, \mathrm{d}s$$

   holds.

The following lemmas can be found as exercises in [16]. See also [59, Lemme 1.1].

Lemma 3.E.5. *Assume* $F : \mathbb{R} \to \mathbb{R}$ *is* $\mathcal{C}^1$*, with* F' *bounded. Suppose* $u \in W^{1,p}(\Omega)$ *for some* $1 \le p \le \infty$*. Then*

$$v := F(u) \in W^{1,p}(\Omega) \qquad \textit{and} \qquad \frac{\partial v}{\partial x_j} = F'(u) \frac{\partial u}{\partial x_j}$$

for $j = 1, ..., N$.

See [16, Chap 5, Exercise 16]

Lemma 3.E.6. *Assume* $1 \le p \le \infty$, Ω *is bounded and* $u \in W^{1,p}(\Omega)$*. Then*

1. $|u| \in W^{1,p}(\Omega)$.
2. u^+, $u^- \in W^{1,p}(\Omega)$ *and*

$$\nabla u^+ = \begin{cases} \nabla u & \textit{a.e. on } \{u > 0\} \\ \mathbf{0} & \textit{a.e. on } \{u \le 0\}, \end{cases} \qquad \nabla u^- = \begin{cases} \mathbf{0} & \textit{a.e. on } \{u > 0\} \\ \nabla u & \textit{a.e. on } \{u \le 0\}. \end{cases}$$

3. $\nabla u = \mathbf{0}$ *almost everywhere on the set* $\{u = 0\}$.

See [16, Chap 5, Exercise 17]

Theorem 3.E.7 (Interpolation inequality)**.** *Let* $0 \le s_j < \infty$, $1 \le p_j < \infty$, $j = 0, 1$*. For* $0 \le \theta \le 1$ *put*

$$s = (1-\theta)s_0 + \theta s_1, \quad \frac{1}{p} = \frac{1-\theta}{p_0} + \frac{\theta}{p_1}.$$

Then there exists a constant $C > 0$ *such that*

$$\|f\|_{W^{s,p}(\Omega)} \le C \|f\|^{1-\theta}_{W^{s_0,p_0}(\Omega)} \|f\|^{\theta}_{W^{s_1,p_1}(\Omega)}, \quad f \in W^{s_0,p_0}(\Omega) \cap W^{s_1,p_1}(\Omega).$$

See [47, Theorem 1.48] or [39, Remarque 9.1] for the case $p = p_0 = p_1 = 2$.

3.F Embeddings

For two normed vector spaces X, Y, with $X \subset Y$ we write $X \hookrightarrow Y$ if the identity $\mathrm{id} : X \to Y$, $\mathrm{id}(x) = x$ is continuous, and $X \subset\subset Y$ if id is compact.

Theorem 3.F.1. *Let $1 \le p \le \infty$ and $\Omega \subset \mathbb{R}^N$ be a bounded Lipschitz domain. For $0 \le k < N/p$ set*

$$p^* = \frac{Np}{N - kp}.$$

1. *For $k \ge 0$ the following embeddings are continuous*

$$
\begin{aligned}
&W^{k,p}(\Omega) \hookrightarrow L^{p^*}(\Omega) && \text{if } k < \frac{N}{p}, \\
&W^{k,p}(\Omega) \hookrightarrow L^{q}(\Omega) && \text{for all } p \in [1,\infty) \quad \text{if } k = \frac{N}{p}, \\
&W^{k,p}(\Omega) \hookrightarrow \mathcal{C}^{0,k-N/p}(\Omega) && \text{if } \frac{N}{p} < k < \frac{N}{p} + 1, \\
&W^{k,p}(\Omega) \hookrightarrow \mathcal{C}^{0,\alpha}(\Omega) && \text{for all } \alpha \in (0,1) \quad \text{if } k = \frac{N}{p} + 1, \\
&W^{k,p}(\Omega) \hookrightarrow \mathcal{C}^{0,1}(\Omega) && \text{if } k > \frac{N}{p} + 1,
\end{aligned}
$$

2. *For $k > 0$ the following embeddings are compact*

$$
\begin{aligned}
&W^{k,p}(\Omega) \subset\subset L^{q}(\Omega) && \text{for all } q \in [1,p^*) \quad \text{if } k < \frac{N}{p}, \\
&W^{k,p}(\Omega) \subset\subset L^{q}(\Omega) && \text{for all } q \in [1,\infty) \quad \text{if } k = \frac{N}{p}, \\
&W^{k,p}(\Omega) \subset\subset \mathcal{C}(\overline{\Omega}) && \text{if } k > \frac{N}{p},
\end{aligned}
$$

Theorem 3.F.1 is stated in [47, 1.3.5.8]. For the case where k is a positive integer, see [1, 5.4 Theorem] and [2, 8.9, 8.13]. For arbitrary positive k and $p < N$, the embeddings of the form $W^{k,p}(\Omega) \hookrightarrow L^q(\Omega)$ are shown in [1, 7.57 Theorem]. Embeddings of the form $H^l(\Omega) \hookrightarrow C^{k,\alpha}$, $H^l(\Omega) \subset\subset C^{k,\alpha}$ or $H^{l_1}(\Omega) \subset\subset H^{l_2}(\Omega)$, $0 \le l_2 < l_1$ can be found in [66, §§6, 7]. See also [25, Theorem 1.4.3.2] for the embedding $W^{s',p}(\Omega) \subset\subset W^{s'',p}(\Omega)$, $s' > s'' \ge 0$.

Theorem 3.F.2 ([54, Section 8, Corollary 4]). *Let $X \subset\subset B \hookrightarrow Y$; X, B, Y be Banach spaces.*

1. *Assume $F = \{f\}$ is bounded in $L^p(0,T;X)$, $1 \le p < \infty$, and $F_t = \{f_t \mid f \in F\}$ is bounded in $L^1(0,T;Y)$. Then F is relatively compact in $L^p(0,T;B)$.*
2. *Let F be bounded in $L^\infty(0,T;X)$ and F_t be bounded in $L^r(0,T;Y)$, $r > 1$. Then F is relatively compact in $\mathcal{C}([0,T];B)$.*

Definition 3.F.3 (Scalar continuity). *Let Y be a Banach space, Y' its dual space, $T > 0$. A function $f : [0,T] \to Y$ is called scalar continuous if the function $\langle y' ; f(t)\rangle : [0,T] \to \mathbb{C}$ is continuous on $[0,T]$, for all $y' \in Y'$.*

Theorem 3.F.4 ([39, Lemme 8.1]). *Be X, Y be two Banach spaces, $X \subset Y$ with continuous injection, X be reflexive. Set*

$$\mathcal{C}_s(0,T;Y) = \{f \in L^\infty(0,T;Y) \ : \ f \text{ scalar continuous of } [0,T] \to Y\}\,.$$

Then it holds: $L^\infty(0,T;X) \cap C_s(0,T;Y) = C_s(0,T;X)$.

Theorem 3.F.5. *Let $T > 0$, $p > 1$, V be a reflexive and separable Banach space, and H be a Hilbert space where V is dense in H with continuous injection $V \subset H$. Define $X := L^p(0,T;V)$, and $W := \{f \in X \ : \ f' \in X'\}$ where $X' = L^{p'}(0,T;V')$ is the dual space of X. Then it holds $W \subset \mathcal{C}(0,T;H)$. For u, $v \in W$ the following formula holds true*

$$\langle u(t)\,,\, v(t)\rangle_{H\times H} - \langle u(s)\,,\, v(s)\rangle_{H\times H} = \int_s^t \Big[\big\langle u'(\tau)\,,\, v(\tau)\big\rangle_{V'\times V} + \big\langle v'(\tau)\,,\, u(\tau)\big\rangle_{V'\times V}\Big]\,\mathrm{d}\tau,$$

for $s,t \in [0,T]$.

Proof. See [23, Chapter IV, §1, Theorem 1.17]. For the case $p = 2$ see also [66, Theorem 25.5] □

3.G Results on the solvability of PDEs

3.G.1 Elliptic problems

Let $\Omega \subset \mathbb{R}^N$ be open and bounded, and let the functions b, $a_{ij} \in L^\infty(\Omega)$, h_i, $f \in L^2(\Omega)$, $i,j = 1,...,N$ be given. Consider the Dirichlet problem

$$\begin{aligned} &\int_\Omega \left[\sum_{i=1}^N \frac{\partial \zeta}{\partial x_i} \cdot \left(\sum_{j=1}^N a_{ij}\frac{\partial u}{\partial x_j} + h_i\right) + \zeta(b\,u + f)\right]\mathrm{d}\boldsymbol{x} = 0 \qquad \text{for all } \zeta \in H_0^1(\Omega), \\ &\qquad\qquad\qquad\qquad\qquad\qquad u \in H_0^1(\Omega). \end{aligned} \tag{3.177}$$

If there exists $c_0 > 0$, such that

$$\sum_{i,j=1}^N a_{ij}(\boldsymbol{x})\,\xi_i\,\xi_j \geq c_0\,|\boldsymbol{\xi}|^2 \qquad \text{for all } \boldsymbol{x} \in \Omega \text{ and } \boldsymbol{\xi} \in \mathbb{R}^N, \tag{3.178}$$

then $(a_{ij}(\boldsymbol{x}))_{i,j}$ is said to be uniformly (in $\boldsymbol{x}$) elliptic.

Theorem 3.G.1 ([2, 4.8]). *Let $b \geq 0$ and (3.178) be satisfied. Then, there exists a unique weak solution $u \in H_0^1(\Omega)$ of problem (3.177). It holds*

$$\|u\|_{H^1(\Omega)} \leq C(\|h\|_{L^2(\Omega)} + \|f\|_{L^2(\Omega)}),$$

where C is an independent of h and f constant.

Theorem 3.G.2 ([2, Theorems A 10.2, A 10.3])**.** *Let $\Omega \subset \mathbb{R}^N$ be open and bounded with Lipschitz boundary, and $u \in H^1(\Omega)$ be the weak solution of the homogeneous Dirichlet problem*

$$\begin{aligned} \sum_{i=1}^{N} \frac{\partial}{\partial x_j} \left(\sum_{j=1}^{N} a_{ij} \frac{\partial u}{\partial x_j} + q_i \right) &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

with $(a_{ij}(\boldsymbol{x}))_{i,j}$ bounded and uniformly elliptic. Suppose $m \geq 0$ and $f \in H^m(\Omega)$, $q_i \in H^{m+1}(\Omega)$, $a_{ij} \in \mathcal{C}^{m,1}(\Omega)$. Then $u \in H^{m+2}(\Omega)_{\mathrm{loc}}$, and $H^{m+2}(D)$-norm of u can be estimated can be estimated by the data, for every open $D \subset \Omega$, with $\overline{D}$ compact.

If $\partial\Omega$ can locally be expressed as the graph of a $\mathcal{C}^{m+1,1}$ function and $a_{ij} \in \mathcal{C}^{m,1}(\overline{\Omega})$. Then $u \in H^{m+2}(\Omega)$, and the $H^{m+2}(\Omega)$-norm of u can be estimated by the data.

Lemma 3.G.3 (The Lamé system)**.** *If Ω is a bounded $(1,1)$-smooth domain, $\mu, \xi > 0$, $\boldsymbol{f} \in L^2(\Omega)^N$, $\boldsymbol{g} \in H^{3/2}(\partial\Omega)^N$. Then the boundary value problem*

$$\begin{aligned} \big[-\mu\Delta - \xi\nabla\mathrm{div}\big]\boldsymbol{U} &= \boldsymbol{f} \quad \text{in } \Omega, \\ \boldsymbol{U} &= \boldsymbol{g} \quad \text{on } \partial\Omega \end{aligned}$$

has a unique weak solution $\boldsymbol{U} \in H^2(\Omega)^N$.

Proof. By Theorem 3.E.2, there exists $\boldsymbol{U}_b \in H^2(\Omega)^N$ with $\boldsymbol{U}_b|_{\partial\Omega} = \boldsymbol{g}$. Therefore, $\boldsymbol{F} = \boldsymbol{f} + [\mu\Delta + \xi\nabla\mathrm{div}]\boldsymbol{U}_b \in L^2(\Omega)^N$, and the problem can be rewritten for $\boldsymbol{u} = \boldsymbol{U} - \boldsymbol{U}_b$ with homogeneous boundary conditions

$$\begin{aligned} \big[-\mu\Delta - \xi\nabla\mathrm{div}\big]\boldsymbol{u} &= \boldsymbol{F} \quad \text{in } \Omega, \\ \boldsymbol{u} &= \boldsymbol{0} \quad \text{on } \partial\Omega. \end{aligned} \tag{3.179}$$

One easily checks that $[-\mu\Delta - \xi\nabla\mathrm{div}]$ is uniformly elliptic, and that the requirements of (the vectorial versions of) theorems 3.G.1 and 3.G.2 are satisfied for $m = 0$. Therefore, (3.179) has a unique weak solution $\boldsymbol{u} \in H^2(\Omega)^N \cap H_0^1(\Omega)^N$, and $\boldsymbol{U} = \boldsymbol{u} + \boldsymbol{U}_b \in H^2(\Omega)^N$ is the asserted solution of the original problem. □

Lemma 3.G.4 (Eigen-values of the Lameé system, see [47, Lemma 4.33])**.** *Let $\Omega \in \mathcal{C}^2$ be a bounded domain. Then there exist countable sets*

$$\begin{aligned} &\{\lambda_j\}_{j=1}^{\infty} \subset (0, \infty), \quad 0 < \lambda_1 \leq \lambda_2 \leq \ldots \\ &\{\boldsymbol{\psi}_j\}_{j=1}^{\infty} \subset H_0^1(\Omega)^N \cap H^2(\Omega)^N \end{aligned}$$

such that

$$-\Delta\boldsymbol{\psi}_j - \nabla\mathrm{div}\,\boldsymbol{\psi}_j = \lambda_j \boldsymbol{\psi}_j$$

and $\{\boldsymbol{\psi}_j\}_{j=1}^{\infty}$ is orthonormal basis $L^2(\Omega)^N$ with respect to the scalar product $\int_\Omega \boldsymbol{u} \cdot \boldsymbol{v}$ as well as an orthogonal basis of $H_0^1(\Omega)^N$ with respect to the scalar product $\int_\Omega [\mu\nabla\boldsymbol{u} : \nabla\boldsymbol{v} + \xi\mathrm{div}\,(\boldsymbol{u}) \cdot \mathrm{div}\,(\boldsymbol{v})]$.

3.G.2 Monotone operators

Definition 3.G.5. *Let V be a Banach space and let the operator $A:\ V \to V'$ be given.*

1. *A is called hemi-continuous if the function $\lambda \mapsto \langle A(u+\lambda v)\,,\, w\rangle$ is continuous from $\mathbb{R} \to \mathbb{R}$ for all $u,\ v,\ w \in V$.*
2. *A is called monotone if the inequality $\langle A(u) - A(v)\,,\, u - v\rangle \geq 0$ holds for all $u,\ v \in V$.*

Definition 3.G.6. *Let V be a reflexive and separable Banach space. An operator $A:\ V \to V'$ is called of the type of "Calculus of Variations", if it is bounded and can be represented by*

$$A(v) = A(v, v),$$

where $u, v \to A(u, v)$ is an operator from $V \times V \to V'$ having the properties:

1. *$\forall u \in V,\ v \mapsto A(u, v)$ is hemi-continuous and bounded from $V \to V'$, and $\langle A(u,u) - A(u,v)\,,\, u - v\rangle \geq 0$.*
2. *$\forall v \in V,\ u \mapsto A(u, v)$ is bounded and hemi-continuous from $V \to V'$.*
3. *If $u_j \rightharpoonup u$ weakly in V and $\langle A(u_j, u_j) - A(u_j, u)\,,\, u_j - u\rangle \to 0$, then $\forall v \in V,\ A(u_j, v) \rightharpoonup A(u, v)$ weakly in V'.*
4. *If $u_j \rightharpoonup u$ weakly in V and $A(u_j, v) \rightharpoonup \phi$ weakly in V', then $\langle A(u_j, v),\, u_j\rangle \to \langle \phi, u\rangle$.*

Lemma 3.G.7 ([38, Chapter. 2.2, Corollaire 2.1])**.** *Let $f \in V'$ be arbitrary, and assume that the operator $A:V \to V'$ is of the type of Calculus of Variations in the sense of Definition 3.G.6. Then, the equation $A(u) = f$ has a solution (at least one).*

3.H The conservation of mass

In this section, we give the results from [56] which are used in Section 3.3 for the investigation of the transport problem. Let us fix the notation notation. Suppose $\Omega \subset \mathbb{R}^N$, $N \in \{2, 3\}$, is a bounded domain with $\mathcal{C}^2$ boundary, and, for $T > 0$, define $Q_T := \Omega \times [0, T] \subset \mathbb{R}^{N+1}$. For a vector field $\boldsymbol{v} : Q_T \to \mathbb{R}^N$ denote by v_i, $i = 1, \ldots, N$ the components of $\boldsymbol{v}$. If $v_i \in L^1_{\text{loc}}(\Omega)$, $i = 1, \ldots, N$, then let $\nabla\boldsymbol{v}$ denote the vector whose components are all of the first-order (distributional) derivatives $\partial_{x_j} v_i$, $i, j = 1, \ldots, N$, and $\nabla^2\boldsymbol{v}$ denote the vector whose components are all of the second-order derivatives $\partial_{x_k}\partial_{x_j} v_i$, $i, j, k = 1, \ldots, N$. Denote the norm in $L^q(\Omega)$ by $\|\cdot\|_{q,\Omega}$ if $q < \infty$ and by $|\cdot|_\Omega$ if $q = \infty$. If $v_i \in L^q(Q_T)$, $i = 1, \ldots, N$, set $\|\boldsymbol{v}\|_{q,Q_T} = \left(\int_{Q_T} |\boldsymbol{v}(\boldsymbol{x}, t)|^q \,\mathrm{d}\boldsymbol{x}\mathrm{d}t\right)^{1/q}$. The spaces $W^{2,1}_q(Q_T)$ and $W^{1,1}_{q,\infty}(Q_T)$ can be defined for $q > N$ as the closures of the sets of (vector)-functions from $\mathcal{C}^2(\overline{Q_T})$, with the norms

$$\|\boldsymbol{v}\|^{(2,1)}_{q,Q_T} = \left\|\nabla^2\boldsymbol{v}\right\|_{q,Q_T} + \|\nabla\boldsymbol{v}\|_{q,Q_T} + \|\boldsymbol{v}_t\|_{q,Q_T} + \|\boldsymbol{v}\|_{q,Q_T}\,,$$
$$\|\rho\|^{(1,1)}_{q,\infty,Q_T} = \sup_{t\leq T}\|\nabla\rho(t)\|_{q,Q_T} + \sup_{t\leq T}\|\rho_t(t)\|_{q,Q_T} + |\rho|_{Q_T}\,.$$

For a given $\boldsymbol{v} \in W_q^{2,1}(Q_T)$, consider the following problem

$$\begin{aligned} \rho_t + \operatorname{div}(\rho\, \boldsymbol{v}) &= 0, \qquad \text{in } Q_T, \\ \rho(0, \boldsymbol{x}) &= \rho^0(\boldsymbol{x}), \quad \text{in } \Omega. \end{aligned} \tag{3.180}$$

To obtain the solution ρ of problem (3.180), consider the characteristic equations defined by the Cauchy problem

$$\frac{\partial \boldsymbol{y}}{\partial \tau}(\tau,\, t,\, \boldsymbol{x}) = \boldsymbol{v}(\boldsymbol{y}(\tau,\, t,\, \boldsymbol{x}),\, \tau)\ , \qquad \boldsymbol{y}(\tau,\, t,\, \boldsymbol{x}) = \boldsymbol{x}. \tag{3.181}$$

Problem (3.181) is uniquely solvable for any $\boldsymbol{v} \in W_q^{2,1}$, $q > N$, which vanishes on $\partial\Omega$. A solution $\boldsymbol{y}$ satisfies the following estimates

$$\begin{aligned} |\nabla \boldsymbol{y}|^2 &= \sum_{j,k}^{N} \left(\frac{\partial y_j}{\partial x_k}\right)^2 \le N \exp\left(2 \int_0^t |\nabla \boldsymbol{v}(\tau)|_\Omega \, \mathrm{d}\tau\right)\ , \\ \left|\frac{\partial \boldsymbol{y}}{\partial t}\right| &\le \sqrt{N}\, |\boldsymbol{V}|_{Q_t} \exp\left(\int_0^t |\nabla \boldsymbol{v}(\tau)|_\Omega \, \mathrm{d}\tau\right) \end{aligned} \tag{3.182}$$

and the relation

$$\boldsymbol{y}_t + (\boldsymbol{V} \cdot \nabla)\boldsymbol{y} = \boldsymbol{0}. \tag{3.183}$$

The next theorem establishes the solvability of problem (3.181) and gives some estimates of the solution ρ. To formulate the theorem, introduce the norm in the space of Hölder continuous functions with the exponent $\alpha \in (0,1)$ by the relations

$$|\rho|_\Omega^{(\alpha)} = |\rho|_\Omega + [\rho]_\Omega^{(\alpha)}, \qquad [\rho]_\Omega^{(\alpha)} = \sup_{\boldsymbol{x},\boldsymbol{y} \in \Omega} \frac{|\rho(\boldsymbol{x}) - \rho(\boldsymbol{y})|}{|\boldsymbol{x} - \boldsymbol{y}|^\alpha}.$$

Theorem 3.H.1 ([56, Theorem 2])**.** *Let $\boldsymbol{v} \in W_q^{2,1}(Q_T)$. For any ρ^0 satisfying the conditions $0 < m_0 \le \rho^0(\boldsymbol{x}) \le M_0$ and $\nabla\rho^0 \in L^q(\Omega)^N$, problem* (3.180) *has a unique solution*

$$\rho(\boldsymbol{x}, t) = \rho^0\left(\boldsymbol{y}(0, t, \boldsymbol{x})\right) \exp\left(\int_0^t \operatorname{div}\left(\boldsymbol{v}(\boldsymbol{y}(\tau, t, \boldsymbol{x}),\, \tau)\right)\, \mathrm{d}\tau\right)$$

from the class $W_{q,\infty}^{1,1}(Q_T)$, for which we have the estimates

$$m_0 \exp\left(-\sqrt{N} \int_0^t |\nabla \boldsymbol{v}(\tau)|_\Omega \, \mathrm{d}\tau\right) \le \rho(\boldsymbol{x}, t) \le M_0 \exp\left(\sqrt{N} \int_0^t |\nabla \boldsymbol{v}(\tau)|_\Omega \, \mathrm{d}\tau\right),$$

$$\begin{aligned} \|\nabla \rho(t)\|_{q,\,\Omega} \le \sqrt{N} &\exp\left([2 + 1/q]\sqrt{N} \int_0^t |\nabla \boldsymbol{v}(\tau)|_\Omega \, \mathrm{d}\tau\right) \\ &\times \left[\|\rho^0\|_{q,\,\Omega} + |\rho^0|_\Omega \sqrt{N} \int_0^t \|\nabla^2 \boldsymbol{v}(\tau)\|_{q,\,\Omega} \, \mathrm{d}\tau\right], \end{aligned}$$

$$\begin{aligned} [\rho(t)]_\Omega^\alpha \le \sqrt{N} &\left[[\rho^0]_\Omega^\alpha + |\rho^0|_\Omega \sqrt{N} \int_0^t [\nabla \boldsymbol{v}(\tau)]_\Omega^\alpha \, \mathrm{d}\tau\right] \\ &\times \exp\left((1 + \alpha)\sqrt{N} \int_0^t |\nabla \boldsymbol{v}(\tau)|_\Omega \, \mathrm{d}\tau\right), \qquad \alpha \in (0,1). \end{aligned}$$

4 Numerical Simulations

In this chapter, problem (2.3) is solved numerically. During the derivation of the equations the density and the surface mass density were denoted by ρ_p and η_p, respectively, to distinguish the particle variables from the flow variables. Due to the assumption of weak compressibility of the liquid, no confusion occurs if p is omitted (the density of the liquid is denoted by ρ_0). Using this notation and the representation of the stress tensor (2.22), we obtain the following initial-boundary value problem

$$\begin{aligned}
\gamma\, p_t + \operatorname{div} \boldsymbol{U} &= 0 && \text{in } \Omega \times (0,T),\\
\rho_t + \operatorname{div}(\rho \boldsymbol{U}) - \beta\, \Delta\rho &= 0 && \text{in } \Omega \times (0,T),\\
\rho_0\, \boldsymbol{U}_t + \operatorname{div}(\boldsymbol{U} \otimes [(\rho+\rho_0)\boldsymbol{U} - \beta\nabla\rho]) &= \boldsymbol{f} + \operatorname{div}\Pi && \text{in } \Omega \times (0,T),\\
\boldsymbol{U} &= \boldsymbol{U}_b && \text{on } \partial\Omega \times (0,T),\\
-[\rho\, \boldsymbol{U}_b - \beta\,\nabla\rho]\cdot \boldsymbol{\nu} &= -g\, \boldsymbol{U}_b \cdot \boldsymbol{\nu} && \text{on } \Gamma^{\text{in}} \times (0,T),\\
-\partial_{\boldsymbol{\nu}}\rho &= 0 && \text{on } \partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}}),\\
-\beta\, \partial_{\boldsymbol{\nu}}\rho = \eta_t, \quad \eta &= \mathcal{A}(\rho) && \text{on } \Gamma \times (0,T),\\
\boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{U}^0(\boldsymbol{x}), \quad p(\boldsymbol{x},0) = p^0(\boldsymbol{x}), \quad \rho(\boldsymbol{x},0) &= \rho^0(\boldsymbol{x}) && \text{for } t=0 \text{ in } \Omega,\\
\eta(\boldsymbol{x},0) &= \eta^0(\boldsymbol{x}) && \text{for } t=0 \text{ in } \Gamma.
\end{aligned} \tag{4.1}$$

This chapter is structured as follows. In Section 4.1, we present a scheme for the numerical solution of problem (4.1) by means of the finite element method (FEM). The results of simulations are given in Section 4.2.

Remark 4.0.2. *As mentioned in Section 1.2, the wet cell developed at CAESAR was constructed to work with organic molecules immersed in water. It should be noted that the diffusion coefficient for organic molecules in water is sufficiently larger than that for rigid particles. An organic molecule is a chain consisting of many links connected by flexible bonds so that the molecule can assume different configurations with a large frequency. This yields hydrodynamical forces that cause relatively large and frequent displacements of the molecule from its average position. Such an effect can be interpreted as a diffusion with a relatively large diffusion coefficient. Simulations presented in [43] and theoretical issues of [34] indicate the presence of such effects. Thus, the diffusion coefficient for organic molecules in water is expected to be much larger than the value for rigid particles in water given in Table 2.6.4. A reasonable guess for the magnitude of the diffusion coefficient yields its value between* 10^{-10} *and* $10^{-8}\,\mathrm{m}^2\cdot\mathrm{s}^{-1}$. *Thus, we will use the value* $10^{-8}\,\mathrm{m}^2\cdot\mathrm{s}^{-1}$ *for our simulation.*

4.1 Discretization scheme

To solve problem (4.1) numerically, we use the finite element program Felics developed at the Chair of Mathematical Modeling at the Technical University of Munich. We propose a discretization scheme that first computes the variables $\boldsymbol{U}$ and p corresponding to the flow of the liquid, and then the variables ρ and η corresponding to the particles. The scheme is obtained as follows.

Let $[0, T]$ be the time interval where the evolution of the mixture is considered. To discretize the time, choose two numbers $m,\ K \in \mathbb{N}$ such that $K/m \in \mathbb{N}$. Define the time step length $\tau := T/K$ and choose a partition $t_0 = 0 < t_1 < t_2 < \cdots < t_{K-1} < t_K = T$ where $t_n = n \cdot \tau,\ n = 1, ..., K$. Denote the unknown velocity, pressure, particle density, and surface mass density of the particles at time $t = t_n$ by $\boldsymbol{U}^n$, p^n, ρ^n, and η^n, respectively. The variables $\boldsymbol{U}^n$ and p^n will be computed only at times t_n with $n = m \cdot j,\ j \in \{1, ..., K/m\}$.

In order to obtain a time discretization of system (4.1), replace the derivatives ρ_t and η_t at time t_n by the difference quotients $(\rho^n - \rho^{n-1})/\tau$ and $(\eta^n - \eta^{n-1})/\tau$, and replace the derivatives $\boldsymbol{U}_t$ and p_t by $(\boldsymbol{U}^n - \boldsymbol{U}^{n-m})/(m\,\tau)$ and $(p^n - p^{n-m})/(m\,\tau)$ to obtain

$$
\begin{aligned}
\gamma \frac{p^n - p^{n-m}}{m\tau} + \operatorname{div} \boldsymbol{U}^n &= 0, \\
\rho_0 \frac{\boldsymbol{U}^n - \boldsymbol{U}^{n-m}}{m\tau} - \operatorname{div} \Pi^n &= \boldsymbol{f}^n - \operatorname{div} C^{n-m}, \\
\frac{\rho^n - \rho^{n-1}}{\tau} - \beta\Delta\rho^n &= -\operatorname{div}\left(\rho^{n-1}\,\boldsymbol{U}^n\right), \\
\boldsymbol{U}^n &= \boldsymbol{U}_b && \text{on } \partial\Omega, \\
-[\rho^n\,\boldsymbol{U}_b - \beta\nabla\rho^n]\cdot\boldsymbol{\nu} &= -g\,\boldsymbol{U}_b\cdot\boldsymbol{\nu} && \text{on } \Gamma^{\text{in}}, \\
-\partial_{\boldsymbol{\nu}}\rho^n &= 0 && \text{on } \partial\Omega \setminus (\Gamma \cup \Gamma^{\text{in}}), \\
-\beta\,\partial_{\boldsymbol{\nu}}\rho^n = \frac{\eta^n - \eta^{n-1}}{\tau}, \quad \eta^n &= \mathcal{A}(\rho^n) && \text{on } \Gamma.
\end{aligned}
\tag{4.2}
$$

The convective term is abbreviated by

$$
C^j = \boldsymbol{U}^j \otimes [(\rho^j + \rho_0)\boldsymbol{U}^j - \beta\nabla\rho^j]. \tag{4.3}
$$

To compute the unknowns in each time step, problem (4.2) is split in the following way. To compute the velocity and pressure at time $t = t_n,\ n = j \cdot m$, assume that $\boldsymbol{U}^{n-m}$, p^{n-m}, ρ^{n-m}, and η^{n-m} are already known. Then $\boldsymbol{U}^n$ and p^n are determined by the subproblem

$$
\begin{aligned}
\gamma \frac{p^n - p^{n-m}}{m\,\tau} + \operatorname{div} \boldsymbol{U}^n &= 0, \\
\rho_0 \frac{\boldsymbol{U}^n - \boldsymbol{U}^{n-m}}{m\,\tau} + \nabla p^n - \mu\Delta\boldsymbol{U}^n - \xi\nabla\operatorname{div} \boldsymbol{U}^n &= \boldsymbol{f}^n - \operatorname{div} C^{n-m}, \\
\boldsymbol{U}^n &= \boldsymbol{U}_b \qquad \text{on } \partial\Omega.
\end{aligned}
\tag{4.4}
$$

To compute the unknowns ρ^n and η^n for $n = (j-1)m+1, ..., j\,m$, assume that (4.4) is already solved for $\boldsymbol{U}^{jm}$, p^{jm}, and the functions ρ^{n-1}, η^{n-1} are already known. Then, the equation of

(4.2) describing the particle variables ρ^n and η^n reads

$$\begin{aligned}\frac{\rho^n - \rho^{n-1}}{\tau} - \beta\Delta\rho^n &= -\mathrm{div}\left(\rho^{n-1}\boldsymbol{U}^{jm}\right), \\ -[\rho^n\boldsymbol{U}_b - \beta\nabla\rho^n]\cdot\boldsymbol{\nu} &= -g\,\boldsymbol{U}_b\cdot\boldsymbol{\nu} && \text{on } \Gamma^{\mathrm{in}}, \\ -\partial_{\boldsymbol{\nu}}\rho^n &= 0 && \text{on } \partial\Omega\setminus(\Gamma\cup\Gamma^{\mathrm{in}}), \\ -\beta\,\partial_{\boldsymbol{\nu}}\rho^n = \frac{\eta^n - \eta^{n-1}}{\tau}, \quad \eta^n &= \mathcal{A}(\rho^n) && \text{on } \Gamma.\end{aligned} \tag{4.5}$$

In the next two sections, we describe an iterative scheme for solving (4.4) and (4.5). Section 4.1.1 contains the treatment of problem (4.5). The presented scheme is the same as in [4]. In Section 4.1.2, a scheme with two intermediate steps presented in [6, 60] is adopted (see also [3]) to solve the flow problem (4.4). In [6, 60] the flow of incompressible fluids is considered. The convergence of approximate velocities and pressures constructed by the scheme to some solution of Navier-Stokes equations is considered in [60, Theorems 7.1 and 7.2].

4.1.1 Discretization of the particle system

The scheme for solving (4.5) is taken from [4]. We will apply it to a weak form of (4.5) because it is suitable for the numerical treatment by means of the finite element method. Assume that the velocity $\boldsymbol{U}^{jm}$ is known for a $j \in \{1,\dots,K/m\}$, and let the particle density ρ^{n-1}, and the surface mass density η^{n-1} be already computed for a $n \in \{(j-1)m+1, ..., j\cdot m\}$. Then, the weak form of (4.5) is given by

$$\begin{aligned}\int_\Omega \left[\left(\rho^n + \tau\,\boldsymbol{U}^{jm}\cdot\nabla\rho^n\right)\psi + \tau\nabla\rho^n\cdot\nabla\psi\right]\mathrm{d}\boldsymbol{x} + \tau\int_{\Gamma^{\mathrm{in}}}\rho^n\,\psi\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s \\ = \int_\Omega \rho^{n-1}\psi\,\mathrm{d}\boldsymbol{x} + \tau\int_{\Gamma^{\mathrm{in}}} g\,\psi\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s - \int_\Gamma\left(\eta^n - \eta^{n-1}\right)\psi\,\mathrm{d}s.\end{aligned} \tag{4.6}$$

Note that the problems (4.5) and (4.6) are similar to (3.87) and (3.90), respectively.

Equation (4.6) contains the two unknowns ρ^n and η^n. To eliminate η^n, rewrite the relation $\eta = \mathcal{A}(\rho)$ in the discrete form (similar to (3.89)):

$$\eta^n(\boldsymbol{x}) - \eta^{n-1}(\boldsymbol{x}) = \left(H(\rho^n(\boldsymbol{x})) - \eta^{n-1}(\boldsymbol{x})\right)^+. \tag{4.7}$$

To resolve the nonlinearity in (4.7), we construct a fixed-point scheme for ρ^n. Note that (4.7) is equivalent to the relation

$$\left(H(\rho^n(\boldsymbol{x})) - \eta^{n-1}(\boldsymbol{x})\right)^+ = h(\rho^n)(\boldsymbol{x})\cdot\left[H(\rho^n)(\boldsymbol{x}) - \eta^{n-1}(\boldsymbol{x})\right], \tag{4.8}$$

where

$$h(\rho^n)(\boldsymbol{x}) = \begin{cases} 0 & \text{if } H(\rho^n)(\boldsymbol{x}) - \eta^{n-1}(\boldsymbol{x}) \le 0, \\ 1 & \text{if } H(\rho^n)(\boldsymbol{x}) - \eta^{n-1}(\boldsymbol{x}) > 0. \end{cases}$$

To construct a fixed-point iteration scheme, choose a small $c > 0$, and rewrite (4.8) as

$$\begin{aligned}\left(H(\rho^n) - \eta^{n-1}\right)^+ &= \left(H(\rho^n)\frac{\rho^n + c}{\rho^n + c} - \eta^{n-1}\right)^+ \\ &= h(\rho^n)\left[H(\rho^n)\frac{\rho^n}{\rho^n + c} - \left(\eta^{n-1} - H(\rho^n)\frac{c}{\rho^n + c}\right)\right].\end{aligned} \tag{4.9}$$

By Lemma 3.4.25, $\rho^n \geq 0$ a.e. in Ω so that $(\rho^n + c)^{-1}$ is well-defined. Substituting the identities (4.7) and (4.9) into (4.6) yields

$$\begin{aligned} &\int_\Omega [\rho^n \psi + \tau \nabla \rho^n \cdot \nabla \psi] + \int_\Gamma \frac{h(\rho^n) \cdot H(\rho^n)}{\rho^n + c} \rho^n \psi \, \mathrm{d}s + \tau \int_{\Gamma^{\text{in}}} \rho^n \psi \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\ &\quad = \int_\Omega \psi \left[\rho^{n-1} - \tau \boldsymbol{U}^{jm} \cdot \nabla \rho^n\right] + \tau \int_{\Gamma^{\text{in}}} g \, \psi \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\ &\quad - \int_\Gamma h(\rho^n) \left(\eta^{n-1} - H(\rho^n) \frac{c}{\rho^n + c}\right) \psi \, \mathrm{d}s. \end{aligned} \tag{4.10}$$

Equation (4.10) can be used to compute a sequence $\{\tilde{\rho}^k\}$ approximating ρ^n. Replacing every appearance of ρ^n either by $\tilde{\rho}^k$ or $\tilde{\rho}^{k-1}$, one can obtain the following recursion scheme:

$$\tilde{\rho}^0 = \rho^{n-1},$$

$$\begin{aligned} &\int_\Omega \left[\tilde{\rho}^k \psi + \tau \nabla \tilde{\rho}^k \cdot \nabla \psi\right] + \int_\Gamma \frac{h(\tilde{\rho}^{k-1}) \cdot H(\tilde{\rho}^{k-1})}{\tilde{\rho}^{k-1} + c} \tilde{\rho}^k \psi \, \mathrm{d}s + \tau \int_{\Gamma^{\text{in}}} \tilde{\rho}^k \psi \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\ &\quad = \int_\Omega \psi \left[\rho^{n-1} - \tau \boldsymbol{U}^{jm} \cdot \nabla \tilde{\rho}^{k-1}\right] + \tau \int_{\Gamma^{\text{in}}} g \, \psi \, |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\ &\quad - \int_\Gamma h(\tilde{\rho}^{k-1}) \left(\eta^{n-1} - H(\tilde{\rho}^{k-1}) \frac{c}{\tilde{\rho}^{k-1} + c}\right) \psi \, \mathrm{d}s. \end{aligned} \tag{4.11}$$

Iterate (4.11) until $\left\|\tilde{\rho}^k - \tilde{\rho}^{k-1}\right\|_{L^\infty(\Omega)}$ is smaller than a specified tolerance and set $\rho^n := \tilde{\rho}^k$.

4.1.2 Discretization of the flow problem

To solve (4.4), we adopt schemes with two intermediate steps suggested in [6, 60] for the numerical treatment of incompressible flow. Assume $n = m \cdot j$ for a $j \in \{1, \ldots, K/m\}$ and define the time step length τ_f for the computation of the flow variables $\boldsymbol{U}^n$ and p^n by $\tau_f = m \cdot \tau$. To use FEM for numerical calculations, problem (4.4) has to be transformed to have homogeneous Dirichlet boundary conditions. Assume the boundary function $\boldsymbol{U}_b$ is extended to $\overline{\Omega}$ such that $\boldsymbol{U}_b \in H^1(\Omega)$ and substitute $\boldsymbol{U}^n = \boldsymbol{u}^n + \boldsymbol{U}_b$ into (4.2). Then, $\boldsymbol{u}^n$ and p^n satisfy the equations

$$\begin{gathered} \gamma \frac{p^n - p^{n-m}}{\tau_f} + \operatorname{div} \boldsymbol{u}^n = -\operatorname{div} \boldsymbol{U}_b, \\ \rho_0 \frac{\boldsymbol{u}^n - \boldsymbol{u}^{n-m}}{\tau_f} - [\mu \Delta + \xi \nabla \operatorname{div}] \boldsymbol{u}^n = \boldsymbol{f}^n - \nabla p^n - \operatorname{div} C^{n-m} + [\mu \Delta + \xi \nabla \operatorname{div}] \boldsymbol{U}_b, \\ \boldsymbol{u}^n \in H_0^1(\Omega)^N, \end{gathered} \tag{4.12}$$

where (4.3) is used to express the convective term.

Remark 4.1.1 (Representation of the pressure)**.** *During the theoretical investigations in Sections 3.4.1 and 3.3.1 we used the continuity equation of* (4.12) *to express the pressure in terms of the initial value and the velocity. For numerical computations, we will use a different method that yields a smoother velocity field. See also Remark 4.1.2.*

To solve (4.12), introduce an auxiliary function $\tilde{\boldsymbol{u}} \in H_0^1(\Omega)^N$ and split the momentum equation of (4.12) into the following two equations:

$$\begin{aligned} \rho_0 \frac{\tilde{\boldsymbol{u}} - \boldsymbol{u}^{n-m}}{\tau_f} - [\mu\Delta + \xi\nabla\mathrm{div}]\,\tilde{\boldsymbol{u}} &= \boldsymbol{f}^n - \mathrm{div}\,C^{n-m} + [\mu\Delta + \xi\nabla\mathrm{div}]\,\boldsymbol{U}_b, \\ \rho_0 \frac{\boldsymbol{u}^n - \tilde{\boldsymbol{u}}}{\tau_f} &= -\nabla p^n. \end{aligned} \tag{4.13}$$

Note that the sum of both equations is the original momentum conservation with $[\mu\Delta+\xi\nabla\mathrm{div}]\boldsymbol{u}^n$ replaced by $[\mu\Delta+\xi\nabla\mathrm{div}]\tilde{\boldsymbol{u}}$. The first equation of (4.13) and the requirement $\tilde{\boldsymbol{u}} \in H_0^1(\Omega)^N$ form an elliptic boundary value problem for $\tilde{\boldsymbol{u}}$. To solve for p^n, proceed as follows. Computing the divergence of both sides of the second equation of (4.13) and using the conservation of mass from (4.12) to eliminate $\mathrm{div}\,\boldsymbol{u}^n$ yields

$$\rho_0\gamma\, p^n - \tau_f^2\,\Delta p^n = \rho_0\gamma\, p^{n-m} - \tau_f\,\rho_0\,\mathrm{div}\,(\tilde{\boldsymbol{u}} + \boldsymbol{U}_b)\,. \tag{4.14}$$

To obtain the boundary condition for (4.14), remember that $\boldsymbol{u}^n = \tilde{\boldsymbol{u}}$ on $\partial\Omega$ and multiply the second equation of (4.13) by the outward normal $\boldsymbol{\nu}$, which yields:

$$-\,\partial_{\boldsymbol{\nu}}\, p^n = 0 \qquad \text{on } \partial\Omega. \tag{4.15}$$

Now the scheme for computing $\boldsymbol{u}^n$ and p^n can be shortly expressed as follows:

1. Solve the first equation of (4.13) to compute the auxiliary velocity field $\tilde{\boldsymbol{u}}$ without accounting for the pressure.
2. Determine the pressure p^n from the problem (4.14), (4.15).
3. Use the last equation of (4.13) to compute a correction for $\tilde{\boldsymbol{u}}$ to obtain $\boldsymbol{u}^n$.

In order to use finite elements, write equations (4.13), (4.14), and (4.15) in the weak form. The auxiliary velocity $\tilde{\boldsymbol{u}}$ is the solutions of the following problem:

$$\begin{aligned} &\tilde{\boldsymbol{u}} \in H_0^1(\Omega)^N, \\ &\int_\Omega [\rho_0\,\tilde{\boldsymbol{u}} + \tau_f\,\mu\nabla\tilde{\boldsymbol{u}} : \nabla\boldsymbol{\psi} + \tau\,\xi\,\mathrm{div}\,\tilde{\boldsymbol{u}}\cdot\mathrm{div}\,\boldsymbol{\psi}]\,\mathrm{d}\boldsymbol{x} \\ &\quad = \int_\Omega \Big[\big(\rho_0\,\boldsymbol{u}^{n-m} + \tau_f\,\boldsymbol{f}^n\big)\cdot\boldsymbol{\psi} \\ &\quad + \tau_f\,\big(C^{n-m} - \mu\nabla\boldsymbol{U}_b\big) : \nabla\boldsymbol{\psi} - \tau_f\,\xi\,\mathrm{div}\,\boldsymbol{U}_b\cdot\mathrm{div}\,\boldsymbol{\psi}\Big]\mathrm{d}\boldsymbol{x} \end{aligned} \tag{4.16}$$

for all $\boldsymbol{\psi} \in H_0^1(\Omega)^N$. The weak form of (4.14) and (4.15) reads:

$$\begin{aligned} &p^n \in H^1(\Omega), \\ &\int_\Omega \big[\rho_0\gamma\, p^n\cdot\phi + \tau_f^2\,\nabla p^n\cdot\nabla\phi\big]\,\mathrm{d}\boldsymbol{x} \\ &\quad = \rho_0\int_\Omega \big[\gamma\, p^{n-m}\cdot\phi - \tau_f\,\mathrm{div}\,(\tilde{\boldsymbol{u}} + \boldsymbol{U}_b)\cdot\mathrm{div}\phi\big]\,\mathrm{d}\boldsymbol{x} \end{aligned} \tag{4.17}$$

for all $\phi \in H^1(\Omega)$. The last equation of (4.13) yields:

$$\boldsymbol{u}^n = \tilde{\boldsymbol{u}} + \frac{\tau}{\rho_0}\,\nabla p^n. \tag{4.18}$$

Remark 4.1.2. *Note that* (4.12) *and* (4.13) *are not exactly the same problems because of the use of* $[-\mu\Delta - \xi\nabla\mathrm{div}]\tilde{\boldsymbol{u}}$ *instead of* $[-\mu\Delta - \xi\nabla\mathrm{div}]\boldsymbol{u}^n$. *Nevertheless, the error introduced this way is of the order* τ_f. *On the other hand, such a trick provides a regularizing effect on the velocity field.*

Moreover, note that the boundary condition (4.15) *for* p^n *is not satisfied by the exact pressure* p *(there is no boundary condition for* p *in* (4.1)*). According to [60, Remark 7.2 and Theorems 7.1 and 7.2], this does not affect the convergence of the scheme when Navier-Stokes equations for incompressible fluids are considered. Thus, we assume that the solutions* p^n *of problem* (4.17) *yield good approximations to the exact pressure (provided that a solution to problem* (4.1) *exists).*

Summarizing the results of Subsections 4.1.1 and 4.1.2, we obtain the following scheme for solving (4.1):

Scheme 4.1.1 Coupled measurement problem

Choose $\epsilon > 0$. Let $K, m \in \mathbb{N}$ be such that $K/m \in \mathbb{N}$.
Set the time step lengths $\tau := T/K$ and $\tau_f := m \cdot \tau$.
Set values for $\boldsymbol{U}^0$, p^0, ρ^0, and η^0.
for $j = 1$ **to** K/m **do**
    Compute the convective term $C^{(j-1)m}$ at $t = (j-1) \cdot \tau_f$ by (4.3).
    Solve (4.16) for the auxiliary velocity $\tilde{\boldsymbol{u}}$.
    Solve (4.17) for the pressure p^{jm} at time $t = j \cdot \tau_f$.
    Compute $\boldsymbol{u}^{jm}$ at time $t = j \cdot \tau_f$ by (4.18).
    Obtain the new velocity $\boldsymbol{U}^j = \boldsymbol{U}_b + \boldsymbol{u}^j$ at time $t = j \cdot \tau_f$.
    for $n = (j-1)m + 1$ **to** $j \cdot m$ **do**
        Set $\tilde{\rho}^0 := \rho^{n-1}$ and $k = 1$.
        repeat
            Solve (4.11) for $\tilde{\rho}^k$.
            Increment $k \leftarrow k + 1$.
        until $\|\tilde{\rho}^k - \tilde{\rho}^{k-1}\| \leq \epsilon$.
        Set the new particle density $\rho^n := \tilde{\rho}^k$.
        Compute η^n by (4.7).
    end for
end for

4.2 Computation results

In this section, numerical computations for the wet cell are presented. For simplicity, we consider spherical titanium dioxide particles. According to Remark 4.0.2, we want to have the diffusion coefficient within the range 10^{-10} to 10^{-8}, which corresponds to titanium dioxide particles in air. From this reason the computations are carried out for $0.01\ \mu\mathrm{m}$ TiO_2 particles not in water but in air. The material constants for air are given in Table 2.6.3 on page 35.

Another parameter that has to be chosen with care is the time step length τ. The examples presented in Section 4.2.1 show that τ has to be relatively small in order to avoid oscillations in the numerical solutions. We will therefore introduce a regularisation of the problem such that computations are not too time-consuming.

Further, the examples presented in Section 4.2.2 show that most of the particles flow through the wet cell without reaching the active part if it is located at the bottom of the wet cell. Thereby, the geometry of the wet cell is modified in order to improve the efficiency of detecting.

The section is structured as follows. In Section 4.2.1, we introduce a regularization of the boundary hysteresis operator. Different configurations of the in- and outlet will be considered in Section 4.2.2. Simulations of a complete model of the wet cell including the introduced regularization are presented in Sections 4.2.3 and 4.2.4 in two and three dimensions.

4.2.1 Regularization of the hysteresis boundary condition

In Section 4.1.2, we already introduced a scheme which produces additional smoothness in the velocity field, for the discretization of the flow problem (4.4), see Remark 4.1.2. Nevertheless, the resulting scheme (see Scheme 4.1.1) is still sensitive with respect to the choice of parameters. The computed results presented in Figures 4.2.2 and 4.2.3 show that an improper choice of the time step can cause oscillations, especially in the surface mass density η.

To handle these effects, we regularize problem (4.1) by adding a parabolic operator with small coefficients to the boundary hysteresis operator. Assume in the following that Γ can be smoothly and isometrically parameterised in terms of two independent space variables (y_1, y_2) if $N = 3$, or one space variable if $N = 2$. Denote the normal to $\partial\Gamma$ with respect to Γ by $\boldsymbol{\nu}_\Gamma$ and the Laplacian on Γ by $\Delta_\Gamma = \partial^2/\partial y_1^2 + \partial^2/\partial y_2^2$. Replace the boundary condition on Γ in (4.1) by

$$\begin{aligned} -\nabla\rho \cdot \boldsymbol{\nu} &= \eta_t + \beta_1 \rho_t - \beta_2 \Delta_\Gamma \rho && \text{in } \Gamma, \\ -\nabla\rho \cdot \boldsymbol{\nu}_\Gamma &= 0 && \text{on } \partial\Gamma, \end{aligned}$$

where β_1, β_2 are small positive numbers. Using this new boundary condition, the weak form (4.6) is replaced by

$$\begin{aligned} &\int_\Omega \left[\left(\rho^n + \tau\, \boldsymbol{U}^{jm} \cdot \nabla \rho^n \right) \psi + \tau\, \nabla\rho^n \cdot \nabla\psi \right] \mathrm{d}\boldsymbol{x} + \tau \int_{\Gamma^{\mathrm{in}}} \rho^n \psi |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\ &\quad = \int_\Omega \rho^{n-1}\, \psi \, \mathrm{d}\boldsymbol{x} + \tau \int_{\Gamma^{\mathrm{in}}} g\, \psi |\boldsymbol{U}_b \cdot \boldsymbol{\nu}| \, \mathrm{d}s \\ &\quad - \int_\Gamma \left[\left(\eta^n - \eta^{n-1} \right) \psi + \beta_1 \left(\rho^n - \rho^{n-1} \right) \psi + \beta_2 \tau\, \nabla_y \rho^n \cdot \nabla_y \psi \right] \, \mathrm{d}s, \end{aligned}$$

where ρ^n and ψ are assumed to be sufficiently regular on Γ, and the components of the gradient $\nabla_y \phi$ of a smooth function ϕ are given by

$$[\nabla_y \phi(\boldsymbol{x})]_j = \sum_{k=1}^{N} \frac{\partial \phi(\boldsymbol{x})}{\partial x_k} \cdot \frac{\partial x_k(\boldsymbol{y}(\boldsymbol{x}))}{\partial y_j} \qquad (j = 1, \ldots, N-1).$$

Proceeding similarly to Section 4.1.1, we obtain the following regularized fixed-point iteration scheme for the approximating sequence $\{\tilde{\rho}^k\}$:

$$
\begin{aligned}
&\tilde{\rho}^0 = \rho^{n-1},\\
&\int_\Omega \left[\tilde{\rho}^k\,\psi + \tau\nabla\tilde{\rho}^k\cdot\nabla\psi\right]\mathrm{d}\boldsymbol{x} + \tau\int_{\Gamma^{\mathrm{in}}}\tilde{\rho}^k\,\psi\,|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\\
&\quad + \int_\Gamma \left[\frac{h(\tilde{\rho}^{k-1})\cdot H(\tilde{\rho}^{k-1})}{\tilde{\rho}^{k-1}+c} + \beta_1\right]\tilde{\rho}^k\cdot\psi\;\mathrm{d}s + \tau\int_\Gamma \beta_2\,\nabla_y\tilde{\rho}_k\cdot\nabla_y\psi\;\mathrm{d}s\\
&\quad = \int_\Omega\left[\rho^{n-1} + \tau\,\boldsymbol{U}^{jm}\cdot\nabla\tilde{\rho}^{k-1}\right]\,\psi\,\mathrm{d}\boldsymbol{x} + \beta_1\int_\Gamma \rho^{n-1}\,\psi\,\mathrm{d}s\\
&\quad + \tau\int_{\Gamma^{\mathrm{in}}} g\,\psi|\boldsymbol{U}_b\cdot\boldsymbol{\nu}|\,\mathrm{d}s\\
&\quad - \int_\Gamma h(\tilde{\rho}^{k-1})\left(\eta^{n-1} - H(\tilde{\rho}^{k-1})\frac{c}{\tilde{\rho}^{k-1}+c}\right)\psi\,\mathrm{d}s,
\end{aligned}
\tag{4.19}
$$

instead of (4.11).

Let us now show the effect of the regularization in a two-dimensional example. Set the data of the problem in (4.1) as follows: $\boldsymbol{U}^0 = \boldsymbol{U}_b = \boldsymbol{0}$, $p^0 = 0$, $\eta^0 = 0$, $\beta = 10^{-3}$, and the initial density ρ^0 as shown in Figure 4.2.1. The diffusion coefficient β is artificially large but suitable to produce the desired effects.

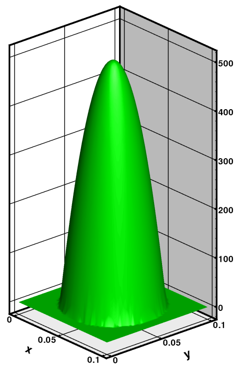


Figure 4.2.1: Inital distribution of particles

The wet cell is assumed to be a two-dimensional rectangle $\Omega = (0,\,0.1)^2$ with the active part located on the bottom $\Gamma = [0, 0.1]\times\{0\}$. To describe the hysteresis operator, the function $H:\mathbb{R}\to[0,1]$ in (2.67) is specified by $\rho_0^* = 0$, $\rho_1^* = 0.1$, and $a = 10$, i.e.

$$
H(s) = \begin{cases} 0 & \text{if } s < 0,\\ 10\,s & \text{if } 0 \le s \le 0.1,\\ 1 & \text{if } s > 1.\end{cases}
$$

The region Ω is discretized by a grid consisting of 3053 points and 5908 triangles. In Scheme 4.1.1, the tolerance for the fixed-point iteration is chosen as $\epsilon = 10^{-4}$.

To compare simulations based on (4.11) and (4.19), three combinations of the parameters β_1, β_2, and τ are used. The unmodified detector corresponds to $\beta_1 = 0$ and $\beta_2 = 0$. The case of regularization is described by $\beta_1 = 1$ and $\beta_2 = \beta$. The time steps are chosen both as $\tau = 5 \cdot 10^{-3}$ and $\tau = 10^{-6}$. We consider the following three cases:

Table 4.2.1: Considered choices of parameters

Parameter	Case 1	Case 2	Case 3
β_1	0	0	1
β_2	0	0	$1\,\mathrm{E}-3$
τ	$5\,\mathrm{E}-3$	$1\,\mathrm{E}-6$	$5\,\mathrm{E}-3$

Figures 4.2.2 and 4.2.3 show numerical results for the particle density and for the saturation of the surface mass density. Since case 2 corresponds to the unmodified detector with the smallest time step, we will consider this result as a quasi-exact reference solution. Figure 4.2.2 shows that the particle densities in all cases are close to each other until the active part is saturated. Comparing cases 1 and 2 in Figure 4.2.2, one can see that a larger time step causes the particle density to rise faster near the saturated region so that a peak in the particle density occurs. One can also see that the density at the active part shows oscillations at later times in case 1. In the case of a smaller time step the particles approaching the saturated part can spread horizontally. Therefore, the density near the boundary remains smaller and smoother in case 2 than in case 1. In case 3, the modified boundary condition oppresses the peak and the oscillations near the saturated parts of the detector, in contrast to case 1. The regularisation also causes a more uniform growth of the particle density near the boundary. Thus, the results of cases 2 and 3 become different when the detector is saturated. Nevertheless, this difference remains smaller than that for cases 1 and 2.

Figure 4.2.3 shows the computed evolution of the surface mass density η on the active part, normalized by the surface mass density $\eta_{\max}$ corresponding to saturation. Similar to the particle density in the wet cell near its active part, the growth of the saturation in case 2 is slower than in case 1. Case 3 shows the slowest growth among the considered cases. The results of case 1 show the largest oscillations, and these oscillations disturb the complete saturation. It should be noted that the shape of the curves is comparable in all cases in spite of kinks caused by oscillations (see Sections 4.2.3 and 4.2.4).

Thus, the comparison of cases 2 and 3 shows that the regularization yields relatively smooth solutions that are close to unregularized ones even for regularization parameters $\beta_1 > \beta$. Further, we will use the regularization in our numerical simulations.

Figure 4.2.2: Computed evolution of the particle density in the cases given by Table 4.2.1

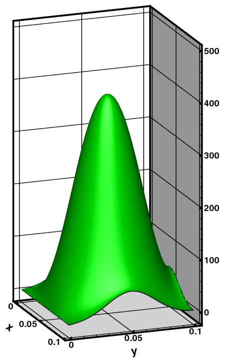
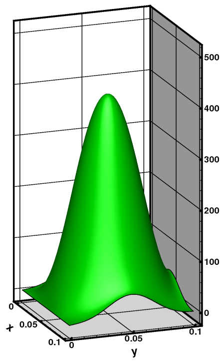
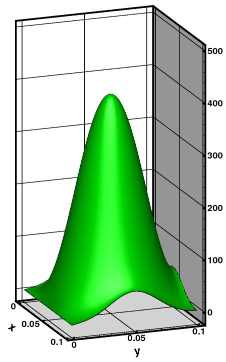
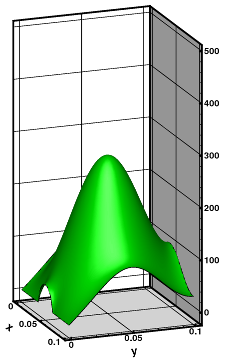
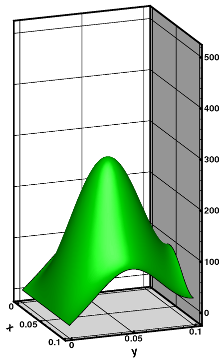
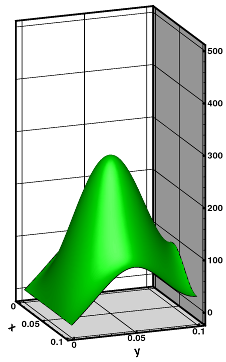
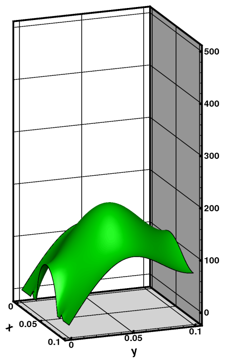
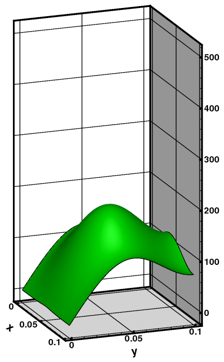
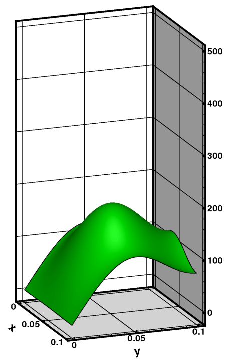
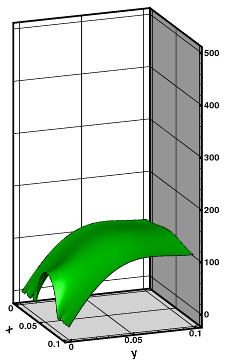
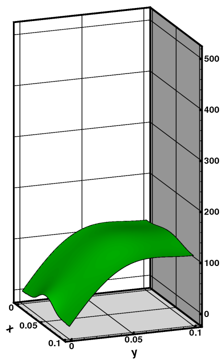
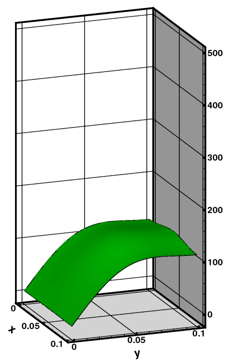
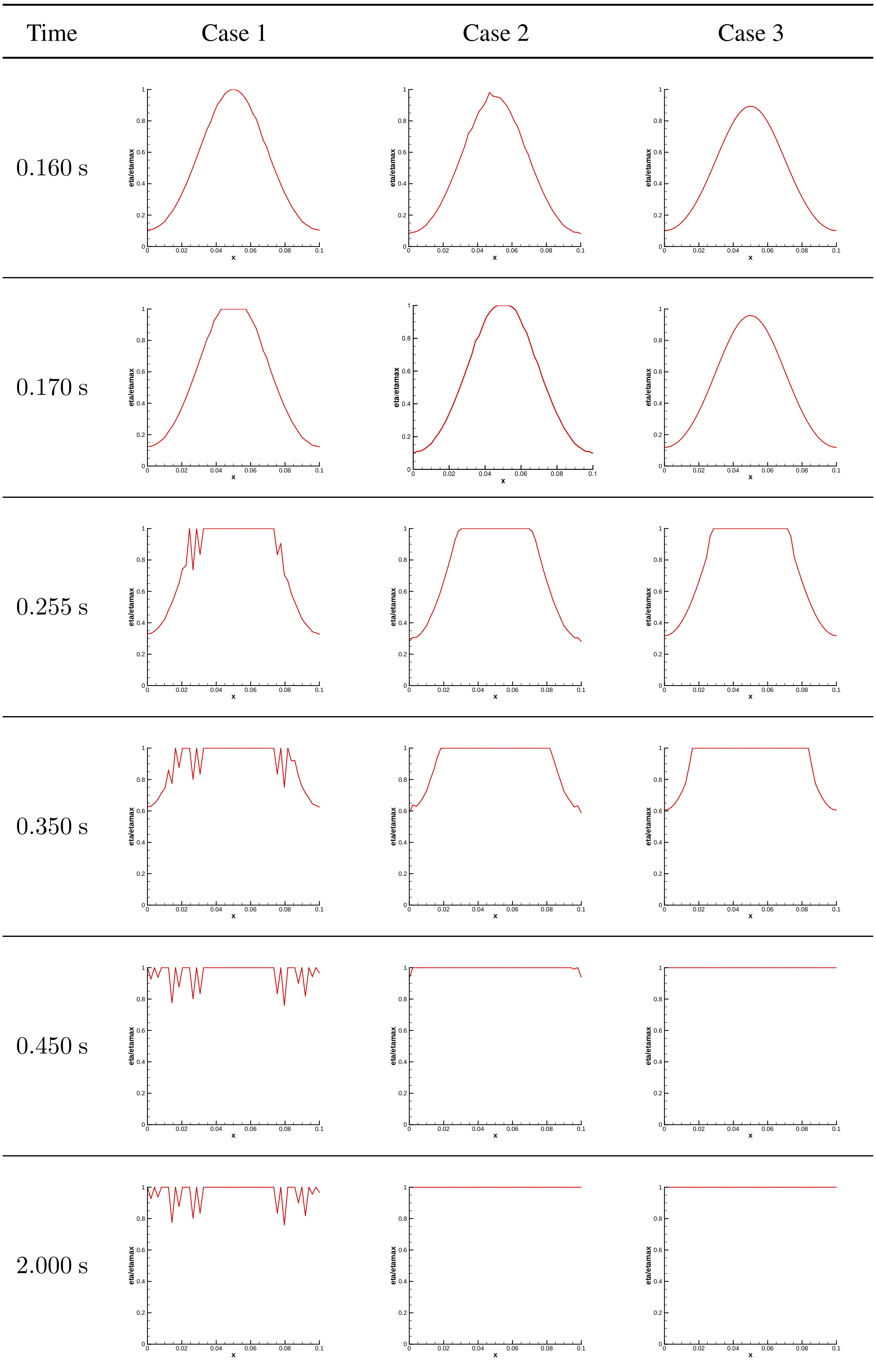
Time	Case 1	Case 2	Case 3
0.075 s			
0.2 s			
0.4 s			
0.8 s			

Figure 4.2.3: Computed evolution of $\eta/\eta_{\max}$ in the cases given by Table 4.2.1

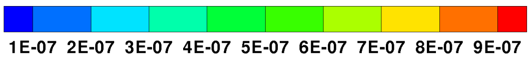
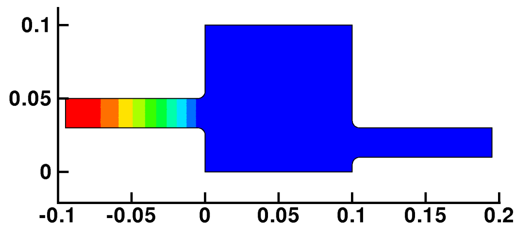
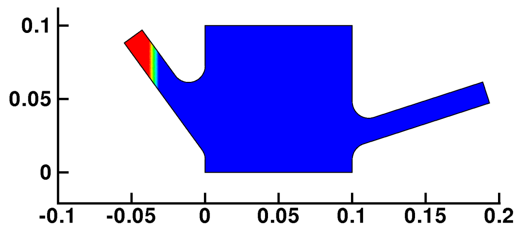
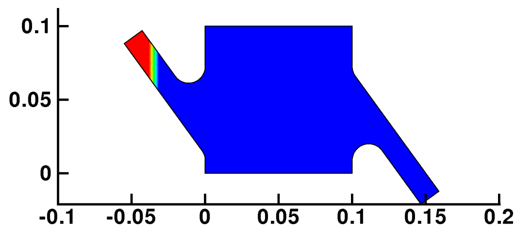


4.2.2 Comparison of geometries

In this section, we consider the motion of particles in the wet cell without active part. Numerical computations show that only a small amount of particles arrives at the bottom of the wet cell in the case of small diffusion coefficients. To show this effect, three numerical experiments with different conditions on the in- and outlet are considered.

The geometry considered in this section is a two dimensional rectangle with the edge length equals $0.1\mathrm{m}$ and with short tubes at the openings. The direction of the tubes models the flow direction on the inlet and outlet. Figure 4.2.4 shows the initial particle density ρ^0 and the considered geometries.

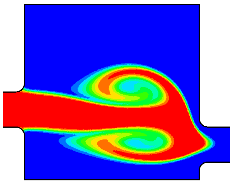
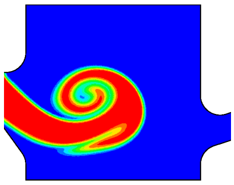
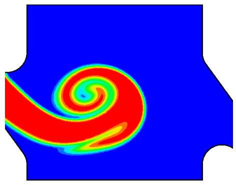
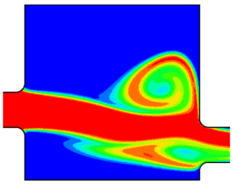
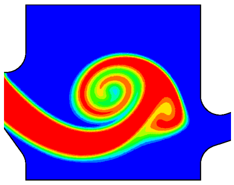
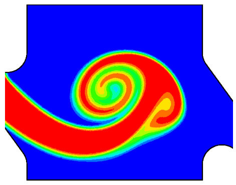
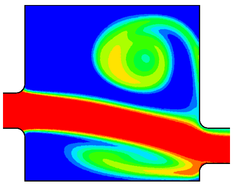
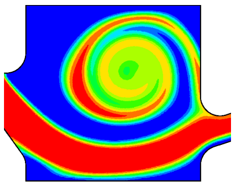
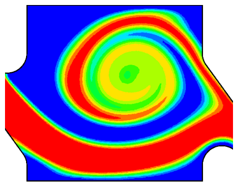
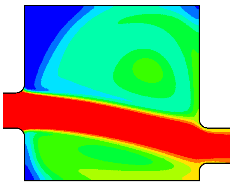
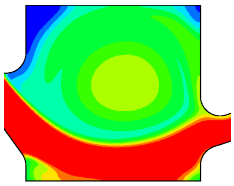
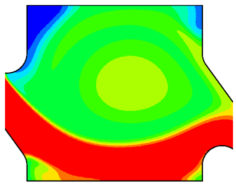
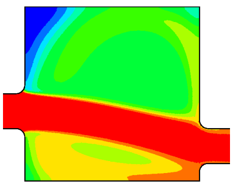
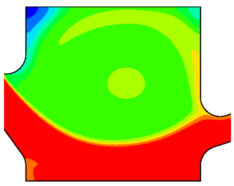
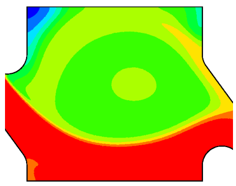
Figure 4.2.4: Geometries and initial conditions for the particle density

Particle density in $\mathrm{kg} \cdot \mathrm{m}^{-3}$:	
Case 1:	
Case 2:	
Case 3:	

In all cases, the boundary function g for the particle density is the trace of ρ^0 on Γ^{in}, the boundary conditions for the velocity is set to $|\boldsymbol{U}_b| = 0.05\mathrm{m/s}$ on Γ^{in} and Γ^{out} in the direction of the tubes, the initial values for the velocity and pressure are $\boldsymbol{U}^0 = \mathbf{0}$ and $p^0 = 0$, and the time steps are $\tau = 10^{-4}\mathrm{s}$ and $\tau_f = 2 \cdot 10^{-3}\mathrm{s}$. The geometry is discretized by grids consisting of about $3 \cdot 10^5$ points and $6 \cdot 10^6$ triangles. The edge length of the triangles is about $7 \cdot 10^{-4}\mathrm{m}$. Actually, the slope of the particle density in case 1 is much smaller than that in other cases. Nevertheless, such a small slope cannot prevent the rapid growth of the gradient in time, see Figure 4.2.5.

The results obtained for the shapes shown in Figure 4.2.4 are presented in Figure 4.2.5. In all cases, the main part of the particles is transported from the incoming tube to the outgoing one without reaching the boundary. The density near the boundary remains small while the majority of particles leaves the sensor. Thus, if the active part is located on the bottom, as it is assumed in the theoretical investigation of Section 3.4.2, it seems difficult to detect a significant amount of particles. The particle density near the bottom as well in the rest of the sensor grows at later times after the formation of a steady state flow regime. For this reason, the geometry of the sensor is changed in Section 4.2.3, and Γ is located on an obstacle in the interior of the wet cell.

Figure 4.2.5: Computed evolution of the particle density in the geometries shown in Figure 4.2.4

Time	Case 1	Case 2	Case 3
3.8 s			
5.0 s			
10.0 s			
40.0 s			
80.0 s			

4.2.3 Simulation in two dimensions

As motivated above, we are changing the geometry of the wet cell to improve the adhesion of particles to the active part. The active part is located on an obstacle in the interior of the wet cell. Thereby, the particles have to flow around the active part before they leave the wet cell.

Figure 4.2.6 shows the new setting and the initial particle density. The wet cell is now supposed to be a rectangle $(0,\, 0.01)^2$, and, as indicated in the figure, the active part Γ is the boundary of the inner circle.

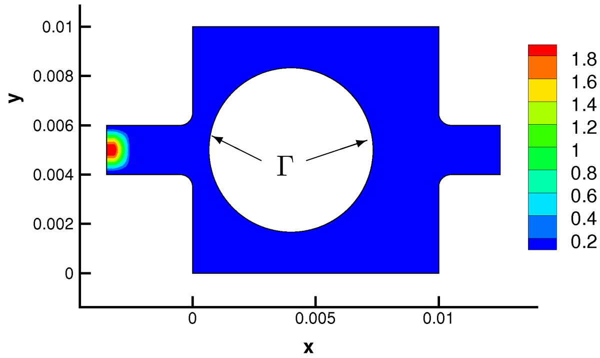


Figure 4.2.6: The modified geometry and initial particle density in units $\mathrm{mg} \cdot \mathrm{m}^{-3}$

The boundary function g on Γ^{in} is the trace of the initial particle density, the velocity at the inlet and outlet is $\boldsymbol{U}_b = \boldsymbol{e}_x \cdot 0.01\ \mathrm{m} \cdot \mathrm{s}^{-1}$ ($\boldsymbol{e}_x$ is the unit vector along the x axis), and the initial functions $\boldsymbol{U}^0$ and p^0 for the velocity and pressure are set to zero. Note that the ratio between the maximal value of the initial distributions in Figures 4.2.1 and 4.2.6 is of order 100. To model the active part analogously to Section 4.2.1, the function H is specified as follows:

$$H(s) = \begin{cases} 0 & \text{if } s < 0, \\ 10\, s & \text{if } 0 \le s \le 0.001, \\ 0.01 & \text{if } s > 0.001. \end{cases} \tag{4.20}$$

The time steps are set to be $\tau = 10^{-5}$ and $\tau_f = 2 \cdot 10^{-3}\,\mathrm{s}$, the tolerance for the fixed-point iteration is $\epsilon = 10^{-3}$, and the regularization parameters are $\beta_1 = \beta_2 = \beta$. To discretize the wet cell a mesh consisting of 8994 points and 17278 triangles is used. That means, the edge length of the triangles is of order $10^{-4}\mathrm{m}$.

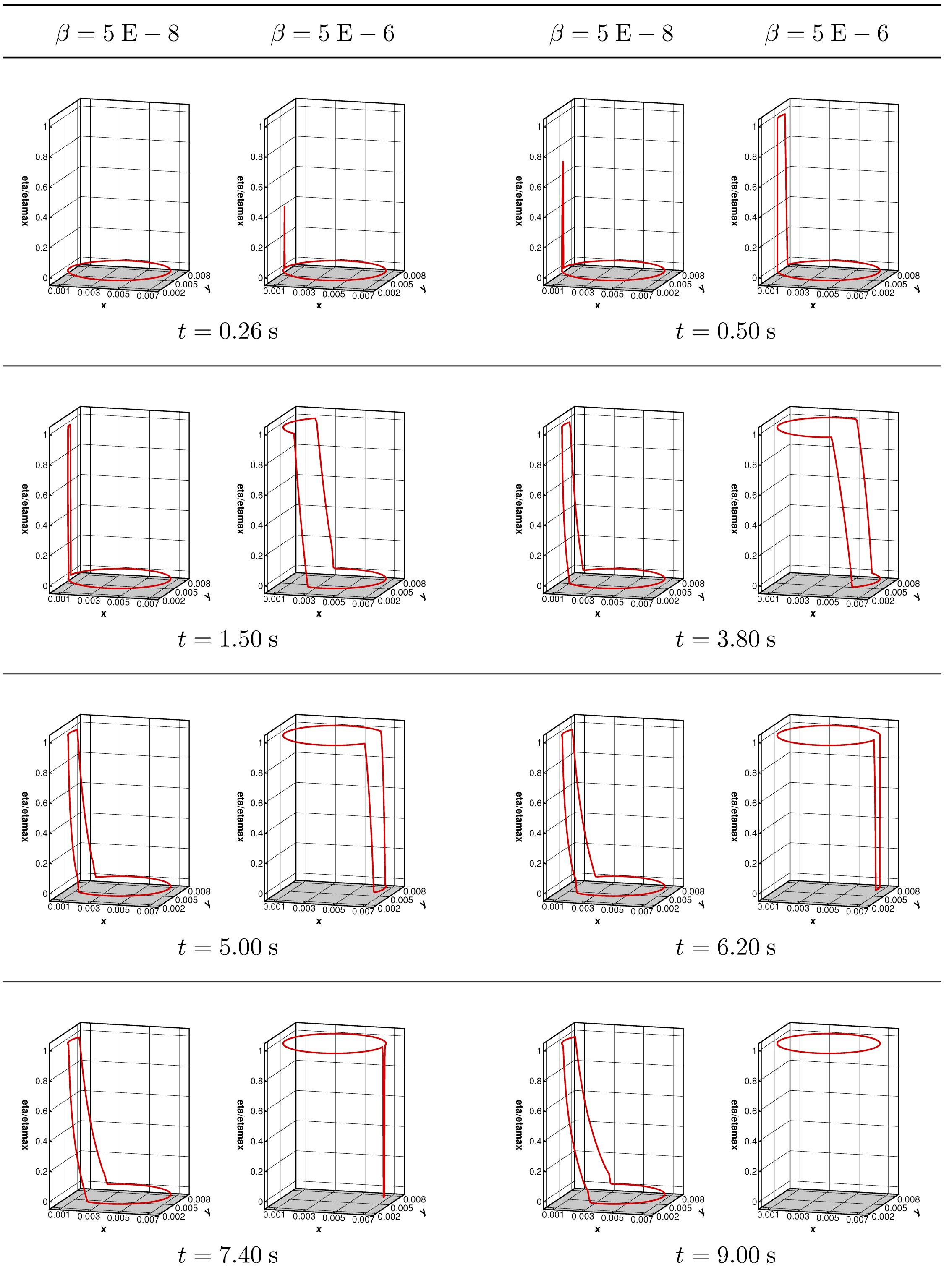
To show the influence of the diffusion coefficient on the evolution of the surface mass density, we compare the results of two simulations with different values of the diffusion coefficient β. In the first computation, we use the diffusion coefficient $\beta = 5 \cdot 10^{-8}\,\mathrm{m}^2 \cdot \mathrm{s}^{-1}$ given in Table 2.6.4, in the second one, we use a larger value of the diffusion coefficient, i.e. $\beta = 5 \cdot 10^{-6}\,\mathrm{m}^2 \cdot \mathrm{s}^{-1}$.

The computed surface mass densities η on the active part, normalized by the surface mass density $\eta_{\max}$ corresponding to saturation, in both cases are compared in Figure 4.2.7. In both cases, a rapid growth of the surface mass density occurs first at the left part of the obstacle. The resulting peak increases and spreads over the active part. The increase stops at those points where the saturation value is reached. As could be expected, the evolution in the case of larger diffusion is quicker, and the whole active part is saturated to the final time instant, whereas the saturation occurs only at the front part of the obstacle in the unmodified setting.

Remark 4.2.1 (Quality of the solutions)**.** *The quality of the numerical solution is yet an open question. For the coupled measurement problem with diffusion coefficients considered in this section, we do not have a reference computation similar to case 2 in Section 4.2.1. Therefore, the deflection from the real solution (if it is unique) cannot be estimated at the moment.*

To interpret the computations, we refer to Section 4.2.1. In the examples considered there, oscillations did not change the shape of the solution dramatically, and the regularized solution was close to that computed with a fine time step. Thus, we hope that the result shown in Figure 4.2.7 is close to the actual solution.

Figure 4.2.7: Computed evolution of $\eta/\eta_{\max}$ on the active part of the wet cell shown in Figure 4.2.6 in the cases $\beta = 5 \cdot 10^{-8}$ and $\beta = 5 \cdot 10^{-6}$



4.2.4 Simulation in three dimensions

In this section, we present a three-dimensional simulation of the wet cell. From the point of view of applications, this is the most interesting case. However, there are many difficulties in the implementation of the numerical algorithm for the problem under consideration – above all, the necessity to use very fine meshes in three dimensions.

The wet cell is supposed to be a cube with edge length equal to 1cm. The active part is located on a cylindrical obstacle (see Figure (4.2.8)). The computed results given in Figure 4.2.7 show that a significant amount of particles can be detected only at the front half of the active part if the value of the diffusion coefficient is $\beta = 5 \cdot 10^{-8}\text{m}^2 \cdot \text{s}^{-1} = 5 \cdot 10^{-4}\text{cm}^2 \cdot \text{s}^{-1}$. Therefore, we consider the geometry shown in Figure 4.2.8 where the active part is shown in red.

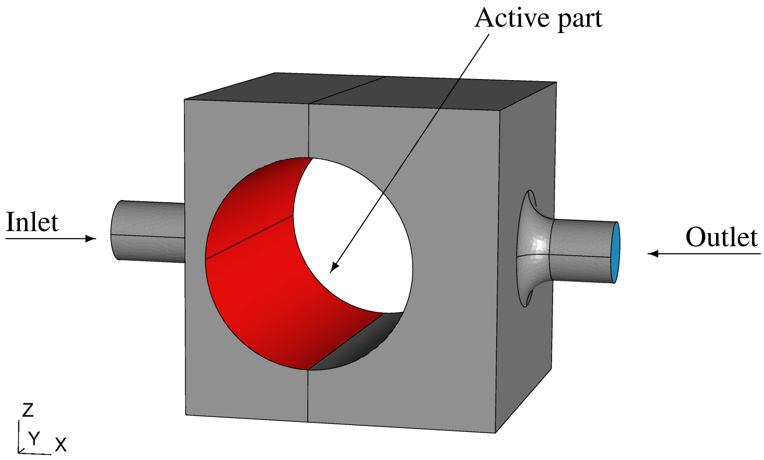


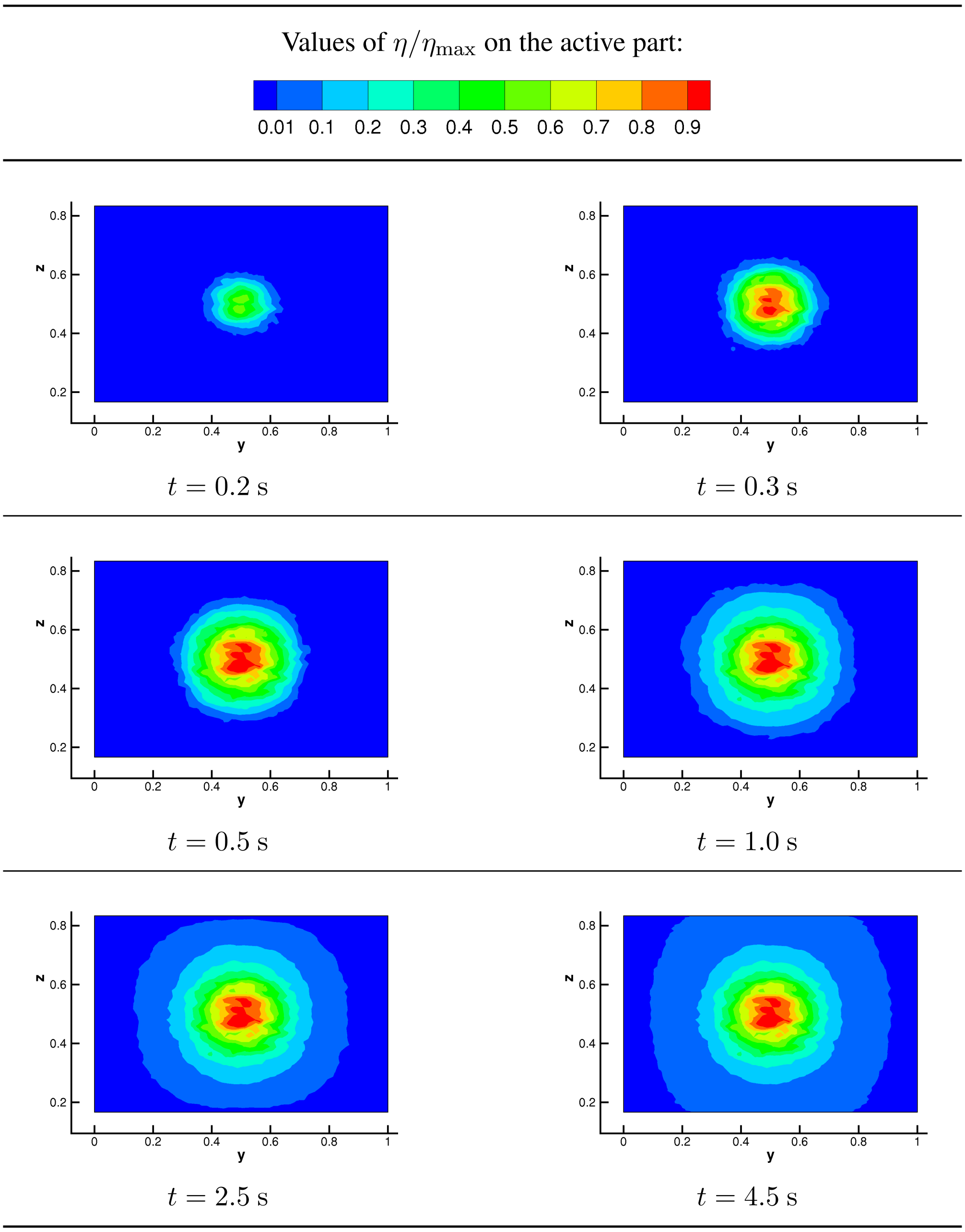
Figure 4.2.8: Geometry of the wet cell in three dimensions

Similarly to Section 4.2.3, the functions $\boldsymbol{U}^0$ and p^0 are set to zero, the boundary value for the velocity is $\boldsymbol{U}_b = \boldsymbol{e}_x \cdot 0.01\text{m/s}$, and the function H is given by (4.20). The initial particle distribution is analogous to that shown in Figure 4.2.4 with its support being extended towards the active part. The boundary function g at the inlet is the trace of the initial particle density. Set the parameters: $\tau_f = 2 \cdot 10^{-3}\text{s}$, $\epsilon = 10^{-3}$ and $\beta_1 = \beta_2 = \beta$. Compared to Section 4.2.3, the time step size and mesh size will be varied. We put $\tau = 5 \cdot 10^{-4}\text{s}$ and use the double mesh size to triangulate the geometry. That means the mesh consists of about $11 \cdot 10^4$ points and $6.6 \cdot 10^5$ tetrahedra with edge length equal to 0.02 cm.

The computed evolution of the surface mass density η, normalized by the surface mass density $\eta_{\max}$, for these parameters and initial and boundary data is shown in Figure 4.2.9. Similar to Figure 4.2.7, the first jump of the surface mass density occurs in the center of the active part, and the resulting peak increases until the saturation is reached. Here the growth of the saturated region stops earlier than in the case of Figure 4.2.7, and the surface mass density of adhered particles increases only at points that lie around the saturated part. In the region where $\eta/\eta_{\max}$ assumes large values, the solution shows oscillations.

As for the quality of the solution, the same situation as in Section 4.2.3 occurs. Because of the absence of the reference simulation similar to that in case 2 of Section 4.2.1, the influence of the introduced regularization and the distance to the real solution has to be considered in future investigations.

Figure 4.2.9: Computed evolution of $\eta/\eta_{\max}$ on the active part of the wet cell shown in Figure 4.2.8



Conclusion

In this thesis, a procedure of detecting small particles dispersed in air is considered. The work is related to investigations (quantitative measurement of nano-particles) carried out at the research institute CEASAR in the course of the European integrated project NANOSAFE2. We consider two problems: transport of particles by air to a washing flask where the particles are being immersed in water and motion of particles in water flowing through a wet cell having an active boundary part responsible for the measurement.

The transport of particles is described by a fully coupled model where particles are considered as a continuum medium. For this problem, the local in time existence and a regularity of generalized solutions are proved. The results obtained are consistent with results for Navier-Stokes equations presented in [36, 56].

For the motion of particles in the wet cell and their adhesion to the active boundary part, another coupled model is derived. The equations describe the evolution of the velocity, pressure, particle density, and surface mass density of measured particles. The specific of the model is a boundary hysteresis operator describing the adhesion of particles and the saturation. For theoretical investigations, the problem is decoupled by neglecting the influence of the particles on the liquid. The existence of weak solutions is proved on a non-empty time interval that depends on the flow problem data. The uniqueness of weak solutions is established in the case where solutions of the flow problem are sufficiently regular. In this case, unique weak solutions of the evolution of the particle density exist on arbitrary time intervals.

A scheme for the numerical treatment of the coupled model of the motion of particles in the wet cell and their adhesion to the active boundary part is proposed. The behavior of the scheme is verified in selected examples. Computational results are presented for two and three dimensions.

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